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Dimensional Strategies and the Minimization Problem: Barrier-Avoiding Algorithms

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In the present paper we examine the role of dimensionality in the minimization problem. Since it has such a powerful influence on the topology of the associated potential energy landscape, we argue that it may prove useful to alter the dimensionality of the space of the original minimization problem. We explore this general idea in the context of finding the minimum energy geometries of Lennard-Jones clusters. We show that it is possible to locate barrier-free, high-dimensional pathways that connect local, three-dimensional cluster minima. The performance of the resulting, "barrier-avoiding minimization" algorithm is examined for clusters containing as many as 55 atoms.

I. Introduction

Perhaps because we instinctively sense that our tools at any moment are, in truth, relatively primitive, we tend to display a reluctance to confront certain issues. Random processes are a case in point. Historically, our view of "noise" was basically that it was "bad". As a consequence, in the past we sought to eradicate, avoid, or minimize it whenever possible. As our abilities to deal with noise have advanced, our views of it have also fundamentally changed. Far from universally avoiding stochastic elements, today we often intentionally introduce them into purely deterministic problems for reasons of "convenience". Random walk treatments of electronic structure[4] and simulated annealing strategies[12,19] for minimization are important examples of this changing perspective.

Years of low-dimensional pedagogy have left an unfortunate legacy. The tendency is to view larger dimensional problems as automatically more difficult than their smaller dimensional counterparts. There are obvious counter examples. Laplace's "two-dimensional" evaluation of the one-dimensional Gaussian integral is a particularly striking one.[13] More recently, advances in formal and computational tools for higher-dimensional systems[3] have contributed to a growing awareness that dimensionality can be transformed from "foe" to "friend".

Dimensionality exerts a powerful influence on phenomenology. The absence of phase transitions in one-dimension[5] and the formal divergence of diffusion coefficients for two-dimensional fluids[1,2] are familiar examples. Because it has such a fundamental influence on the topology of potential energy "landscapes", it is, as suggested by Purisima and Scheraga,[20,21] useful to consider dimensional modification as a tool within the context of the minimization problem.

The present paper examines a particular class of dimensional modification strategies. As a prototype application, we consider the problem of finding the minimum energy geometry of Lennard-Jones clusters. We show that there exist barrierless, higher dimensional pathways that connect three-dimensional, local cluster minima. On the basis of our findings we suggest that dimensional modification may prove to be a useful strategy for certain classes of minimization problems.

The remainder of this paper is organized as follows: Section II introduces the basic idea of dimensional expansion. Results of the application of these methods to Lennard-Jones clusters are presented in Section III. Section IV contains a discussion and summary of the results as well as a comparison with currently available methods.

II. Formal Developments

Minimization problems are arguably among the most ubiquitous in science and engineering. They are also among the most frustrating. What appears to be a relatively simple task for a few variables rapidly becomes quite challenging as the number of degrees of freedom increases. This rise in complexity mirrors the rapid increase of the number of local minima in the associated potential energy landscape with increasing numbers of degrees of freedom. For example, the number of stable local minima increases roughly exponentially with the number of particles for relatively simple Lennard-Jones cluster systems.[22,26] At heart, therefore, the minimization problem is effectively the local minimum problem.

In the present section we explore the potential of dimensionality for use as a tool in the treatment of minimization problems. We examine whether the increase in the complexity of the minimization problem with system size is inevitable or whether it an example of allowing the potential "solution" to become the "problem". We consider conventional minimization techniques only briefly, referring the reader to existing reviews of those methods for more detailed treatments.[19] To provide an explicit framework for our discussion, we adopt the viewpoint throughout the following that the objective function we seek to minimize is a generalized potential energy surface for a realizable physical system whose natural coordinates are continuously variable quantities.

For the present discussion, it is convenient to divide minimization techniques into two broad classes—those that modify the underlying potential energy surface and those that

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do not. Standard conjugate gradient methods as well as various "annealing" approaches[19] fall into the latter category. On the basis of a variety of physically motivated analogies, annealing methods leave the underlying potential energy surface itself unchanged. The most common of these methods, simulated annealing,[12,19] adopts a classical statistical−mechanical point of view. Specifically, the strategy is to locate the potential minimum by following the associated classical probability density as the "temperature" of the system is reduced. If the "cooling schedule" is sufficiently conservative (i.e., if care is taken to ensure that the thermal fluctuations are sufficient to defeat the local minimum problem), the density will ultimately condense onto the global potential minimum in the limit of zero temperature. Unfortunately, however, this procedure can fail in practice. Situations in which differences between the energies of major potential basins are small relative to the barriers that separate them can, for example, prove particularly difficult. By the time it becomes apparent that one is headed toward a local minimum, the scale of the relevant thermal fluctuations can, for computationally feasible cooling schedules, be too small to have any practical chance of overcoming the energy barrier.

Rather than viewing the original objective function as a potential surface for a finite temperature *classical* system, "quantum annealing" methods[6,11] employ a finite temperature, *quantum-mechanical* model. The global minimum of the specified potential is again located by following the density (or ground state wave function) toward the zero-temperature, classical limit. If we perform the limits by first turning off the quantum mechanics and then reducing the temperature, we recover conventional simulated annealing. We are free, however, to reverse the order of the limits, first taking temperature to zero and then turning down the quantum mechanics. There is practical merit to this second approach. Specifically, ground state diffusion Monte Carlo methods[4] provide a general (stochastic!) means for performing the zero-temperature limit not available in purely classical approaches. Once the ground state is reached, the quantum mechanics of the problem can be turned off by, for example, gradually increasing the masses of the particles of the system. In quantum annealing, tunneling, as opposed to thermal fluctuations, provides the mechanism for avoiding local minima. Quantum-mechanical optimization approaches based on a dynamical model have been proposed by Straub et al.[14]

As indicated earlier, annealing methods do not alter the underlying potential energy surface. Quantum annealing does, however, change the way in which information concerning the potential is processed during intermediate stages of the minimization process. While the classical density at a point depends on the potential energy at that specific location, the quantum-mechanical density is influenced by the values of the potential energy throughout a surrounding neighborhood.

A second broad strategy for the design of minimization algorithms involves purposefully modifying the original potential energy surface. That is, rather than simply modifying the way in which potential energy information is processed, we seek to distort the potential in such a way that we obtain an algorithmic advantage while leaving the global minimum essentially intact. Early work by Stillinger and Stillinger[23] is an example of this type of approach. They sought to reduce the number of local minima by altering the long-range form of simple pair potentials. Strategies based on "smoothing" techniques have also been proposed.[18,23] More recently, Wales et al.[10,27] have devised an approach based on a "basin hopping" methodology in which the original potential energy at each point is replaced by the energy of its corresponding local minimum or "inherent structure".[22,24,25] By construction, the basin hopping method, unlike some distortion strategies, is guaranteed to leave the energetics of the various potential minima unaltered. By eliminating or lessening barriers between neighboring inherent structures, however, the approach promotes transitions between various local minima. The procedure is simple to implement and has proved effective in a variety of applications.[7,9,15,16,28]

TABLE 1: Number of Stable Isomers Found for a 13 Atom Lennard-Jones Cluster in Various Dimensions

dimension	*no. of isomers*
1	1
2	345
3	1505
4	363
5	88
6	27
7	16
8	5
9	4
10	2
11	1
12	1

The present work explores another class of minimization strategies. Broadly speaking, the approach is a potential modification technique that combines elements of both basin-hopping and dimensional-relaxation strategies. A simple analogy will suffice to convey the essential idea. As anyone who has ever hiked in the mountains knows, it is often easier to "contour" around a local "barrier" than to climb over it. Rather than blindly restricting ourselves to lower dimensional ridge routes that go over barriers, we seek instead higher dimensional, barrier-free routes that bypass them. In a similar spirit, the present method attempts to defeat the local minimum problem by constructing barrier-free, high-dimensional pathways that connect the various three-dimensional inherent structures.

Why do we have any hope that such high-dimensional pathways either exist or that they will be helpful for the general minimization problem? To answer this basic question, it is useful to first pose another: How many three-dimensional isomers exist for a four-atom Lennard-Jones cluster? A bit of reflection will reveal that the answer to the latter question is one. In three dimensions each of the four atoms can be a nearest neighbor of all of the remaining particles by forming a tetrahedron. Using similar arguments, it is simple to see that an N-particle Lennard-Jones cluster will have a single isomer in $N - 1$ dimensions. Because all atoms can be nearest neighbors of every other atom, it is also simple to see that the energy of this $N - 1$ dimensional, minimum energy structure is less than the energy of any other inherent structure in any number of dimensions.

To make the connection between dimensionality and the number of local minima more explicit, we list in Table 1 the number of energetically distinct isomers found for the 13 atom Lennard-Jones cluster as a function of the number of spatial dimensions. We assume the potential energy of these clusters to be of the pairwise form

$$V(\boldsymbol{R}) = \sum_{i<j} V_{LJ}(|\boldsymbol{r}_i - \boldsymbol{r}_j|) \tag{2.1}$$

where $\boldsymbol{r}_i$, is a D-dimensional vector whose components ($x_{i,1}$, $x_{i,2}$...$x_{i,D}$) specify the position of atom "i". The Lennard-Jones interaction, $V_{LJ}(r)$, specified in terms of the usual well-depth, ϵ, and length scale, σ, parameters by

$$V_{LJ}(\boldsymbol{r}) = 4\epsilon\left[\left(\frac{\sigma}{\boldsymbol{r}}\right)^{12} - \left(\frac{\sigma}{\boldsymbol{r}}\right)^{6}\right] \tag{2.2}$$

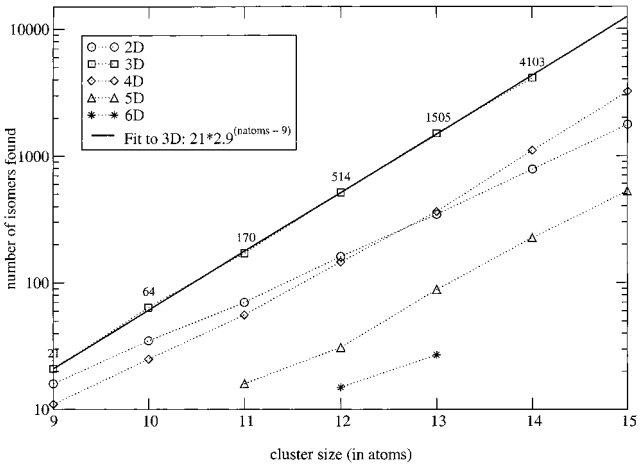

Figure 1. The number of stable isomers found for Lennard-Jones clusters of various sizes in different numbers of dimensions. As discussed in the text, the results are intended to convey the effects of cluster size and dimensionality on the inherent structure topology. Given the uncertainty inherent in attempts to locate all local minima, the numbers shown should be regarded as lower bounds to the exact values. A fit to the number of stable isomers for an N-atom cluster in three dimensions, $I(N) = I(N_0)\Gamma^{N-N_0}$, shows essentially exponential growth relative to a baseline value for 21 isomers for $N_0 = 9$. The fitted value of Γ indicates that the number of stable isomers grows (on average) by roughly a factor of 2.9 with the addition of each new particle. The corresponding two-dimensional value is 2.22.

is a function of the D-dimensional interparticle Euclidian distance, $|\boldsymbol{r}_i - \boldsymbol{r}_j|$,

$$|\boldsymbol{r}_i - \boldsymbol{r}_j| = \left(\sum_{n=1}^{D} (x_{i,n} - x_{j,n})^2\right)^{1/2} \tag{2.3}$$

These results in Table 1 were established by quenching initial configurations produced by a D-dimensional, basin-hopping random walk with standard gradient methods. The resulting structures were tested to ensure they indeed corresponded to stable minima. The number of quenches used is sufficient to identify the general trend with respect to dimensionality (i.e., that the number of stable isomers is a decreasing function of dimensionality above three dimensions). Although we do find slightly more three-dimensional isomers for the 13 atom system than were reported by Tsai and Jordan[26] or by Doye, Miller, and Wales,[8] the results of Table 1 should not in general be taken as definitive with respect to the exact number of stable isomers for any particular cluster and dimension.

Figure 1 charts the growth of the number of isomers of Lennard-Jones clusters from 9 to 15 atoms for various numbers of dimensions. The growth appears roughly exponential in this cluster size range. It is interesting to note that the number of stable isomers for these clusters appears to be a maximum for three-dimensions.

How can we exploit the apparent "simplifying" effect of dimensionality on the cluster's inherent structure topology? One possibility, suggested by Purisima and Scheraga,[20,21] is to start with what we know a priori to be the unique global minimum in $N - 1$ dimensions and attempt to compress that structure back to three dimensions. While appealing, we have not found this approach to be a generally successful one for our applications. The essential difficulty is that dimensional quenches do not appear to link high and low-dimensional global minima in a direct, "adiabatic" fashion.

We have, however, found another, and apparently more general, way to exploit dimensional expansion. From Table 1 and Figure 1, we see that the number of local cluster minima tends to decrease as the dimensionality of the system is increased above three dimensions. In fact, as discussed previously, when the dimensionality is sufficiently large, we know that the number of high-dimensional minima ultimately shrinks to unity. We further know that the energy of this unique, high-dimensional minimum lies below that of any other minimum (local or global) in any number of dimensions. Although these results do not specify how to find it, they guarantee the existence of a barrier-free, $N - 1$ dimensional pathway between any three-dimensional local minimum and the three-dimensional global minimum for an N-particle cluster. To see this result, it is sufficient to note that the three-dimensional local and global minima both are points on a single, $N - 1$ dimensional potential basin. By construction, therefore, there is an $N - 1$ dimensional, barrier-free pathway that connects the designated local and global minima. It is straightforward to generalize this argument to show that any two local, three-dimensional minima are connected by a barrier-free, $N - 1$ dimensional pathway. How large does the dimensionality have to be in practice in order that a barrier-free pathway exist? How general is the simplifying effect of dimensionality on the topology of the high-dimensional inherent structure surface? The answer to the second question awaits further study. On the basis of results presented in the following section, however, it appears that the answer to the first question is, for Lennard-Jones clusters, only slightly greater than three.

III. Numerical Method and Examples

We now describe our implementation of barrier-avoiding minimization and examine its performance for small ($N < 55$ atoms) Lennard-Jones clusters. In part, we have chosen this system for our initial applications because resources like the Cambridge Cluster Database (http://brian.ch.cam.ac.uk) greatly simplify the process of validating the cluster structures and energies that are encountered.

The function we are trying to minimize, $V(\boldsymbol{R})$, is assumed to depend only on the distances between the particles. The class of such functions includes the pairwise additive potentials of the present study, as well as other forms which will be discussed below. In this way, the function is defined for configurations in any dimension; only the definition of the distance changes.

Let D be the dimension (usually 3) in which the original N-particle cluster configuration resides, and H the number of "extra" dimensions to be used in the search. H is useful from 1 to $(N - 1 - D)$. Above this value of H, the $(D + H)$ dimensional atoms only see an $(N - 1)$ dimensional subspace. Given this configuration, we denote the new $(D + H)$ dimensional coordinates by $\boldsymbol{R} = (\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}N)$, where $\boldsymbol{r}_i = (x_{i,1}, x_{i,2}, \ldots, x_{i,D}, x_{i,(D+1)}, \ldots, x_{i,(D+H)})$ and where $x_{i,j}$ is the jth component of the Cartesian coordinates of particle i. We call $\boldsymbol{R}$ D-dimensional (but embedded in a $(D + H)$ dimensional space) if $x_{i,(D+1)} = x_{i,(D+2)}, \ldots, x_{i,(D+H)} = 0$ for all i.

In the algorithm discussed below it is necessary both to expand and compress the cluster between D and $D + H$ dimensions. To execute such expansions and compressions it is essential that we have available a suitable "signature" of the dimensionality of the space. We assume in the following that we have available some suitable "width" function, $W_D(\boldsymbol{R})$, that is continuous in $\boldsymbol{R}$, equal to zero when $\boldsymbol{R}$ is D-dimensional, and otherwise positive. One choice for the width function, the

one used in the present study, is

$$W_D(\boldsymbol{R}) = \sum_{i=1}^{N} \sum_{n=D+1}^{D+H} x_{i,n}^2 \tag{3.1}$$

The basic idea behind the present algorithm is that, given a local minimum in three dimensions, we can find another, three-dimensional structure via a random walk *at constant potential energy* in a higher dimension. That is, we can move from a three-dimensional energy minimum to another energy "basin" using higher dimensional pathways. The new structure is either another local minimum at the same energy as the starting configuration, or it is a new structure that is not a local minimum. If the new structure is energetically degenerate with the starting configuration, we simply continue the search. If, as is much more likely, the new structure is not a local minimum, then we are assured that it can be relaxed to a new local minimum *with a lower energy*. In this way, we produce a sequence of three-dimensional inherent structures of decreasing potential energies leading to the lowest energy three-dimensional structure.

The steps performed by the algorithm are as follows: given an arbitrary starting configuration, $\boldsymbol{R}$;

1. Find the "inherent structure" for $\boldsymbol{R}$. We minimize $V(\boldsymbol{R})$ for $\boldsymbol{R}$ constrained to stay in D dimensions (i.e., the H higher components are zero). Any minimization technique[19] that decreases V is acceptable for this step (e.g., steepest descent, conjugate-gradient, etc.). More formally, given an initial configuration $\boldsymbol{R}_0$, we find $\boldsymbol{R}$ such that:

$$\text{(a)}\ \frac{dV(\boldsymbol{R})}{d\boldsymbol{r}_i} = 0 \text{ for all } \boldsymbol{r}_i$$

$$\text{(b)}\ \frac{d^2V(\boldsymbol{R})}{d\boldsymbol{r}_i d\boldsymbol{r}_j} > 0 \text{ for all } \boldsymbol{r}_i, \boldsymbol{r}_j$$

$$\text{(c)}\ V(\boldsymbol{R}) \le V(\boldsymbol{R}_0)$$

In part (b) we exclude the directions equivalent to overall translation and rotation of the system. We denote the energy of the (local) minimum produced by steps (a−c) E_{LM} and the associated configuration $\boldsymbol{R}_{LM}$.

2. Perform a constant-energy random walk. This walk consists of *nsteps* constrained random displacements of $\boldsymbol{R}$ in $(D + H)$ dimensions, the constraint being $V(\boldsymbol{R}) = E_{LM}$. In the present paper, we generate trial displacements, $\Delta\boldsymbol{R}$, by uniformly translating all particles within a "box" of about 0.1σ. The value of *nsteps* was 100 for the smaller clusters, 50 for the 38 atom cluster, and 30 for the 55 atom cluster.. The constraint was imposed (to first order) by removing the component of $\Delta\boldsymbol{R}$ parallel to the gradient of $V(\boldsymbol{R})$. For large translations, this is not sufficient, and one must either use a higher order correction (involving the Hessian) or, as was done in the present paper, readjust $\Delta\boldsymbol{R}$ by moving parallel to the energy gradient until the constraint is met (rejecting the "trial" $\Delta\boldsymbol{R}$ if the constraint cannot be met this way).

3. Minimize $W_D(\boldsymbol{R})$ while keeping $V(\boldsymbol{R}) = E_{LM}$. Techniques for such minimizations are widely available in the "nonlinear programming" literature.[17] Our technique is to use the strategy outlined in Step (2), but setting $\Delta\boldsymbol{R} = -c \nabla W_D(\boldsymbol{R})$, where c adjusts the step size at each step so that the gradient is followed downhill (with respect to $W_D(\boldsymbol{R})$) to a (constrained) local minimum.

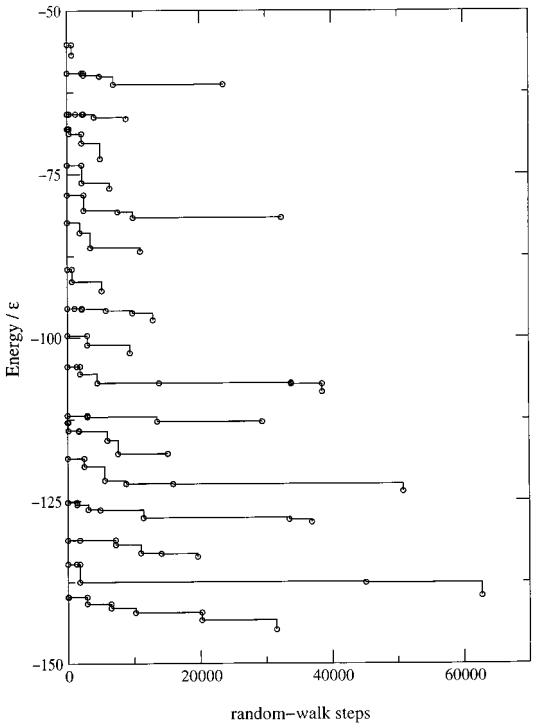

Figure 2. Barrier-avoiding minimization histories for Lennard-Jones clusters containing from 16 to 33 atoms. Starting from a different, randomly chosen configuration for each cluster size, the minimization proceeds, via high-dimensional, barrier-free pathways, through a series of local minima (plateaus in the figure) to the minimum energy configuration. Traces correspond, in order from top to bottom, to results for 16−33 atoms.

4. If the minimization in (3) results in $\boldsymbol{R}$ being D-dimensional (i.e., $W_D(\boldsymbol{R}) = 0$), and $\boldsymbol{R} \neq \boldsymbol{R}_{LM}$, then we may have succeeded in finding a configuration that will quench to a lower energy, D-dimensional inherent structure. In this instance, we start again at Step (1) with the new configuration. By proceeding through a sequence of inherent structures of successively lower energies, we are removing large numbers of local minima from the search as it proceeds.

5. On the other hand, the constrained minimization in (3) can fail in its attempt to "compress" the $(D + H)$ dimensional configuration in Step (2) completely back to D-dimensions. In such cases, we resume our high-dimensional search by resetting $\boldsymbol{R}$ to the last, high-dimensional configuration generated by the random walk in Step (2) and continuing the expanded dimensional walk from that point until Step (4) is satisfied.

We have implemented this "barrier avoiding minimization" procedure and have examined its efficacy for finding the global minima of clusters whose atoms interact via the Lennard-Jones pair-potential. All calculations reported here were done with $H = 1$; that is, the random walk was performed in four dimensions. Although four dimensions proved to be sufficient to produce barrier-free minimization pathways for all examples considered in the present work, it may be necessary to revisit this issue for other applications. We first discuss the cases of 16−33 atoms and then do a more detailed examination of the 38 atom case.

Figure 2 shows the results of a typical set of applications of the barrier avoiding minimization procedure (Steps (1−5) above) for clusters ranging from 16 to 33 atoms. This figure is presented both to convey a sense of the sequence of inherent structure energies visited by the clusters enroute to their global potential energy minima and to illustrate (crudely) the scaling of effort with respect to cluster size. In Figure 2, the minimizations for

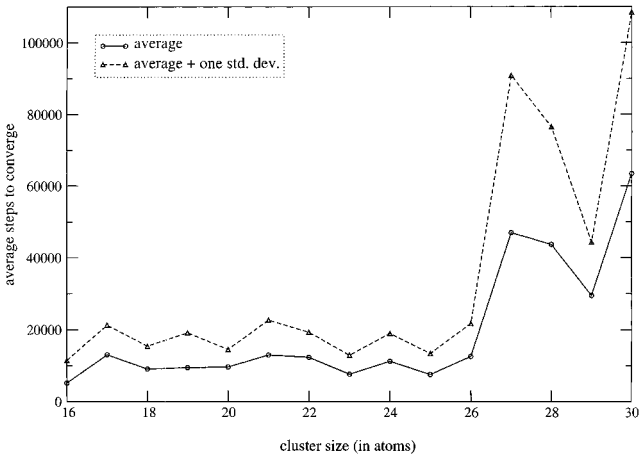

Figure 3. Average number of steps required to reach global minimum for Lennard-Jones clusters of various sizes. The solid (dotted) line represents the average (average plus one standard deviation) of the number of steps required to find the ground state structure for 20 randomly chosen initial configurations for each cluster size.

each cluster size have each been initiated from a single, randomly chosen initial configuration. Figure 3 elaborates upon the issue of the scaling of effort. There we show the average number of steps required to achieve the global potential minima for 20 randomly generated initial configurations for each cluster size. It is first important to note that the present procedure successfully locates the global minima for *all* random initial configurations for *all* cluster sizes. It is also important to note that the level of effort required to find the global minimum energy structure in the range of 16−26 atoms is relatively constant. In particular, over the size range shown in Figure 2, the number of local minima grows (based on exponential fits to the results of Figure 1) by roughly 3×10^6 (from approximately 3.6×10^4 (16 atoms) to 1×10^{11} (30 atoms)). Beyond 26 atoms, the effort required increases, although not prohibitively, as evidenced by our success (see below) with both the 38 and 55 atom clusters. The reasons for this increase in effort are, at present, unclear. It may, however, be an indication that higher dimensional ($H > 1$) minimization pathways could prove useful for studies of larger clusters.

As a somewhat more demanding test of the procedure, we examine its performance for the 38 atom Lennard-Jones cluster. As discussed by Doye, Miller, and Wales,[7] this cluster presents significant challenges in optimization and simulation studies. Its *fcc*-like global minimum is separated from a low-lying, icosohedral local minimum by an appreciable barrier. Figure 4 displays the results of applying the barrier-avoiding minimization method to this system. As illustrated in Figure 4, starting from a randomly generated configuration, the method successfully locates the global minima. It is important to note that the minimization trace shown in Figure 4 actually proceeds through the 38 atom icosohedral local minimum. This is significant in that it confirms that the method did, in fact, locate a barrier-free, four-dimensional pathway "around" what is otherwise a significant, three-dimensional barrier. From Figure 4 we see that in this case roughly 400 000 high-dimensional steps (8000 dimensional quenches) are required to locate the global minimum. The number of quenches for this single minimization is not wildly out of line with the mean first-encounter time of 2000 conjugate-gradient quenches reported for the basin-hopping treatment of the same system.[7]

Finally, although it is a somewhat less challenging example than the 38 atom case, we note that we have also had success

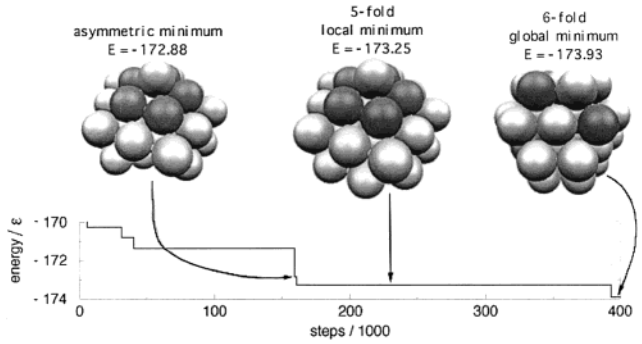

Figure 4. A barrier-avoiding minimization history for the 38 atom Lennard-Jones cluster. The trace shows the results for a single, randomly chosen configuration. It is important to note that the global minimum is reached by way of the icosohedral local minimum. This confirms that the minimization strategy successfully located a barrier-free, high-dimensional pathway from the *fcc* local minimum to the ground-state configuration.

in locating the minimum energy structure for the 55 atom cluster. Systematic studies of larger clusters are planned.

IV. Discussion & Summary

In the present paper, we have explored the use of dimensional strategies for minimization problems. We have presented a particular method that exploits the simplifying influence of dimensionality on inherent structure topology. For one class of systems, Lennard-Jones clusters, we have shown the resulting approach represents a practical minimization method. Using this method, we have succeeded in locating high-dimensional, barrier-free pathways between three-dimensional local minima and the corresponding global minimum-energy structures for clusters containing up to 55 atoms. We are encouraged by the present results, particularly by the method's performance in locating the global minimum for the 38 atom cluster.

In order for the current approach to be of general significance, it will be necessary to establish its utility for a broader range of applications. Although we are cautiously optimistic, the final decision concerning the ultimate fate of the present method must, therefore, await the outcome of ongoing studies.

If dimensional approaches are to be of general merit, two basic conditions must be satisfied. First, it is necessary that dimensionality exert a simplifying effect on the inherent structure topology for the problem of interest. Second, one must find a way to translate this simplification into a practical minimization algorithm. In the present work, both conditions have been met. As discussed in Section II, increasing cluster dimensionality reduces the number of local minima. We have shown, using the barrier-avoiding methods discussed in Section III, how to transform this dimensional simplification into a viable minimization procedure. Although the particular strategy described by Purisima and Scheraga[20,21] for exploiting it does not appear to be general, their work illustrates the important point that the simplifying effects of dimensionality on the minimization problem extend to classes of potentials of chemical interest. Leaving aside the particulars for the moment, the "take-home" message of the present investigation is that whether it is the barrier-avoiding methodology of Section III or some other, yet to be discovered, implementation, dimensional strategies appear to represent a potentially valuable tool for the construction of new classes of minimization algorithms.

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