Parallel Two-Level Simulated Annealing

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Abstract

In this paper, we propose a new kind of simulated annealing algorithm called *two-level simulated annealing* for solving certain class of hard combinatorial optimization problems. This two-level simulated annealing algorithm is less likely to get stuck at a non-global minimizer than conventional simulated annealing algorithms. We also propose a parallel version of our two-level simulated annealing algorithm and discuss its efficiency. This new technique is then applied to the Molecular Conformation problem in 3 dimensional Euclidean space and implemented on the Thinking Machines CM-5. With the full Lennard-Jones potential function, we were able to get satisfactory results for clusters with as many as 100,000 atoms. A peak rate of over 0.8 giga flop per second in 64-bit operations was sustained on a partition with 512 processing elements. To the best of our knowledge, ground states of Lennard-Jones clusters of as large as these have never been reported before.

1 Introduction

Simulated annealing is a general purpose combinatorial optimization technique that has been proposed by Kirkpatrick et al. [19]. This method is an extension of a Monte Carlo method developed by Metropolis et al. [23], to determine the equilibrium states of a collection of atoms at any given temperature T. Since the method was first proposed in [19, 20], much research has been conducted on its use and properties. Some relevant references are: [3, 7, 9, 10, 16, 17, 24, 26].

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In this paper, we present a new kind of simulated annealing algorithm called two-level simulated annealing which is less likely to get stuck at a non-global minimizer. Instead of moving from one solution to another, the two-level simulated annealing algorithm moves from one catchment basin of a local minimizer to the catchment basin of another (or the same) local minimizer. Advantages of this new algorithm over conventional simulated annealing algorithms are discussed. A new method of parallelizing a sequential simulated annealing (conventional or two-level) algorithm is presented next. The parallel algorithm is usually different from the sequential algorithm, but follows the same philosophy of simulated annealing algorithms and is very efficient. These techniques are then applied to the Molecular Conformation problem and implemented in F77 and message passing mode on the Thinking Machines CM-5. The Northby algorithm [25] for Molecular Conformation is combined with our two-level simulated annealing algorithm to get satisfatory results for Molecular Conformation problems of sizes much larger than ever reported before. These computational results demonstrate that the parallel two-level simulated annealing algorithm is a very powerful tool for solving certain class of hard combinatorial optimization problems.

The rest of the paper is organized as follows. In section 2, we present the two-level simulated annealing algorithm and discuss its advantage over conventional simulated annealing algorithms. In section 3, we present a paradigm for parallelizing sequential simulated annealing algorithms. In section 4, we present the Molecular Conformation problem, the combinatorial optimization problem associated with it, and Northby's pivot algorithm for solving the combinatorial optimization problem. In section 5, our parallel two-level simulated annealing algorithm is combined with the Northby algorithm to solve the combinatorial optimization problem in Molecular Conformation. Computational results on the CM-5 are also discussed.

2 Two-Level SA

Given a real-valued function $f(x)$ defined on a feasible domain $\mathcal{D}$, the general global optimization (minimization) problem is to find a point $x^* \in \mathcal{D}$ such that $f(x)$ is globally minimized at x^*, i.e., $f(x^*) \leq f(x)$ for all $x \in \mathcal{D}$. The general global optimization problem is stated as follows.

$$(P) \qquad \begin{array}{ll} \text{global minimize} & f(x), \\ \text{subject to} & x \in \mathcal{D}. \end{array}$$

A point $x^* \in \mathcal{D}$ is called a global minimizer of (P) if $f(x^*) \leq f(x)$ for all $x \in \mathcal{D}$. A point $x^* \in \mathcal{D}$ is called a local minimizer of (P) if $f(x^*) \leq f(x)$ for all x in a neighborhood of x^*. Here we are interested in finding a global minimizer of (P). There have been many approaches to solving (P), e.g., Multistart with Bayesian Stopping Rules [2], Genetic Algorithms [17], and Simulated Annealing [19, 20]. In this paper, we are interested in simulated annealing like algorithms.

The basic simulated annealing algorithm as proposed by Kirkpatrick et al. [19, 20] for solving (P) is stated in Figure 1, where α is a given constant in the interval (0, 1), *number_of_iterations* is a given positive integer, and *perturbation*() is a procedure which generates a new trial point be making a small perturbation from the current solution.

Algorithm_1: Simulated Annealing
Set T to a positive number (initial temperature).
Set x_{old} to an initial feasible solution and compute $f_{old} := f(x_{old})$. Set $x_{best} := x_{old}$ and $f_{best} := f_{old}$.
repeat
  for i := 1 to *number_of_iterations*
    $x_{new} :=$ *perturbation*(x_{old}); $f_{new} := f(x_{new})$;
    generate a random number $r \in (0, 1)$;
    if $((f_{new} \leq f_{old})$ or $(r \leq exp((f_{old} - f_{new})/T)))$ then
      $x_{old} := x_{new}$; $f_{old} := f_{new}$;
      if $(f_{new} < f_{best})$ then
        $x_{best} := x_{new}$; $f_{best} := f_{new}$;
      endif
    endif
  endfor
  $T := \alpha T$;
until (stopping criterion is met)
Output x_{best} and f_{best} as the best known solution and objective function value.

Figure 1: **Basic simulated annealing algorithm**

A simulated annealing algorithm differs from a conventional iterative improvement algorithm in that it not only accepts a solution with better objective function value but also accepts a solution with a worse objective function value conditionally. When the temperature T is high, the probability of accepting a solution with a worse objective function value is relatively large, making it relatively easy for the simulated annealing algorithm to go from the catchment basin corresponding to one local minimizer to the catchment basin corresponding to another local minimizer. It is expected that the algorithm will arrive at the catchment basin of the global minimizer before the temperature T gets very low. When the temperature T gets very low, the algorithm will essentially accept a solution only if the new solution has a better objective function value. Therefore, if the algorithm has already arrived in the catchment basin of a (global or local) minimizer, it will eventually converge to that minimizer.

This method has been proved quite useful in solving hard problems in combinatorial optimization. However, we observe that the simulated annealing algorithm as stated above suffers from certain drawbacks as described in the following scenario: After a large number of iterations (the temperature has already been very low), the algorithm arrives at a strictly local minimizer. Unfortunately, this local minimizer is not a global minimizer. A small perturbation of this local minimizer produces a new solution still in the catchment of this local minimizer. Since the local minimizer is a strict one and that the temperature is low, this move will be rejected. The algorithm tries many times to move in vain, and finally stops at this non-global solution!

In certain optimizations problems, it might be relatively cheap to perform a local minimization from any given feasible points. These are the problems which we are interested in. We will propose a two-level simulated annealing algorithm for solving this kind of optimization problems. It will be seen that the new algorithm is less likely to get stuck in the above scenario than conventional simulated annealing algorithms.

Suppose that we are given problem (P) and a cheap local minimization algorithm. For any given feasible point $x \in \mathcal{D}$, define $\underline{x}$ to be the local minimizer which the given local minimization algorithm will lead to from x. Suppose that a small perturbation from x produces y and that we want to determine whether to accept the move or reject it. The conventional simulated annealing algorithm will compare $f(x)$ and $f(y)$ to make this decision. We think that it is is more meaningful to compare

$f(\underline{x})$ and $f(\underline{y})$ in order to determine whether to accept or reject the move, because we are interested in finding local minimizers and therefore a point lying on a hill is not of our interest. This idea leads to the following two-level simulated annealing algorithm.

Algorithm_2: Two-Level Simulated Annealing
Set T to a positive number (initial temperature). Set x_{old} to an initial feasible solution and compute $\underline{x_{old}}$.
Set $f_{old} := f(\underline{x_{old}})$; $x_{best} := x_{old}$; and $f_{best} := f_{old}$.
repeat
  for i := 1 to *number_of_iterations*;
    $x_{new} := perturbation(x_{old})$; $f_{new} := f(\underline{x_{new}})$;
    generate a random number $r \in (0, 1)$;
    if $((f_{new} \leq f_{old})$ or $(r \leq exp((f_{old} - f_{new})/T)))$ then
      $x_{old} := x_{new}$; $f_{old} := f_{new}$;
      if $(f_{new} < f_{best})$ then
        $x_{best} := x_{new}$; $f_{best} := f_{new}$;
      endif
    endif
  endfor
  $T := \alpha T$;
until (stopping criterion is met)
Output $\underline{x_{best}}$ and f_{best} as the best known solution and objective function value.

Figure 2: **Two-level simulated annealing algorithm**

Our two-level simulated annealing algorithm differs from a conventional simulated annealing algorithm in that it operates on two sequences of iterative points $\{x_k\}$ and $\{\underline{x_k}\}$. We call $\{x_k\}$ the upper level and $\{\underline{x_k}\}$ the lower level for the simple reason that the objective function value of $\underline{x_k}$ is lower than or equal to that of x_k. The perturbation (move) is made on the upper level while the decision of accepting or rejecting the move is based on the comparison of the objective function value on the lower level. Therefore the algorithm is named *two-level simulated annealing.*

Why is a two-level simulated annealing algorithm necessary? Suppose that a small perturbation of x produces y. $f(y)$ may be greater than, equal to, or less than $f(x)$. This information is useful, but not enough. Even more useful information is the answer to the following question: Starting from y, will a local minimization algorithm arrive at a better (lower) local minimizer than $\underline{x}$, a same local minimizer as $\underline{x}$ or a different local minimizer with same objective function value as $\underline{x}$, or a worse local minimizer than $\underline{x}$? The two-level simulated annealing algorithm looks ahead for the latter information before making any decision. In the first two cases, the two-level simulated annealing algorithm will accept the move. In the third case, it will accept the move conditionally, depending on the random number *rand*, the temperature T, and the difference in $f(\underline{x})$ and $f(\underline{y})$. When the temperature T gets very low, the two-level simulated annealing will still accept moves which lead to worse function values, but these moves essentially all lead to better (or same) local minimizers. In other words, the two-level simulated annealing algorithm can easily climb up the hill of a catchment basin of a minimizer at any temperature, but is very careful in moving into the catchment basin of a worse local minimizer when the temperature T is low.

3 Parallel Simulated Annealing

How to implement a (two-level) simulated annealing algorithm efficiently on a given parallel machine?

The easiest way to implement a simulated annealing algorithm on a parallel machine is to parallelize the function evaluation phase of a sequential algorithm. In this case, the parallel algorithm will be the same as the sequential algorithm, except that the function evaluation phase is speeded up. This kind of implementation is not efficient unless the function evaluation is the most significant part of the algorithm and that the function evaluation can be parallelized efficiently.

A second kind of parallel simulated annealing algorithms has been proposed by [7]. There, they present a method for parallelizing the simulated annealing algorithm by mapping the algorithm onto a dynamically structured tree of processors. They have studied the SA Decision Tree and designed three parallel simulated annealing algorithms, namely the Static PSA, the Dynamic Balanced PSA, and the Dynamic Unbalanced PSA. However, the speedup one can hope in the worst case for the Static PSA on a P processor machine is $\log_2 P$. For the other two PSA's, various assumptions are required to guarantee a reasonable speedup. There are many versions of parallel simulated annealing algorithms. We will not try to mention all of them here. In what follows, we will present a parallel (two-level) simulated annealing similar to the one proposed in [10].

We will present our parallel (two-level) simulated annealing algorithm on a EREW MIMD multiprocessors (or tightly coupled machines). This algorithm will be implemented in a master-slave mode on the Thinking Machines CM-5, a SPMD supercomputer (which can be think of as a loosely coupled machines), to solve the Molecular Conformation problem. For terminologies of

parallel computers, readers are referred to [1].

The parallel algorithm that we are going to describe is a nondeterminacy algorithm in the sense that the parallel algorithm is doing different work than the sequential algorithm and that different runs of the program on the same parallel computer will perform slightly different work (especially in a timesharing mode like the CM-5). By no means, we claim that determinacy is not important. We do think, however, that our parallel algorithm is efficient and that it follows the philosophy of (two-level) simulated annealing.

In the following description of our parallel algorithm, T, x_{old}, x_{best}, f_{old}, f_{best}, i, and *done* are global variables. All other variables are local variables, although each processor also has a local variable with the same name for each of the global variables.

Algorithm_3: Parallel Two-Level Simulated Annealing
{Initialize global variables}
Set T to a positive number (initial temperature). Set x_{old} to a initial feasible solution and compute $\underline{x_{old}}$.
Set $f_{old} := f(\underline{x_{old}})$, $x_{best} := x_{old}$, $f_{best} := f_{old}$,
$i := 1$, $done := FALSE$.
repeat_in_parallel
  $lock(done,\ i,\ T,\ f_{old},\ x_{old})$;
  $read(done,\ i,\ T,\ f_{old},\ x_{old})$;
  $unlock(done,\ i,\ T,\ f_{old},\ x_{old})$;
  if $(done = TRUE)$ exit repeat_in_parallel loop
  if $(mod(i, number\_of\_iterations) = 0)$ then
    $lock(T)$; $T := \alpha T$; $unlock(T)$;
  endif
  $lock(i)$; $i := i + 1$; $unlock(i)$;
  $x_{new} := perturbation(x_{old})$; $f_{new} := f(\underline{x_{new}})$;
  generate a random number $r \in (0,\ 1)$;
  if $((f_{new} \leq f_{old})$ or $(r \leq exp((f_{old} - f_{new})/T)))$ then
    $lock(x_{old})$; $x_{old} := x_{new}$; $unlock(x_{old})$;
    $lock(f_{old})$; $f_{old} := f_{new}$; $unlock(f_{old})$;
    $lock(f_{best})$; $read(f_{best})$; $unlock(f_{best})$;
    if $(f_{new} < f_{best})$ then
      $lock(x_{best})$; $x_{best} := x_{new}$; $unlock(x_{best})$;
      $lock(f_{best})$; $f_{best} := f_{new}$; $unlock(f_{best})$;
    endif
  endif
  if (stopping criterion is met) then
    $lock(done)$; $done := TRUE$; $unlock(done)$;
  endif
endrepeat
Output x_{best} and f_{best} as the best known solution and objective function value.

Figure 3: Parallel two-level simulated annealing

It should be clear from the description of the algorithm that two runs of the same algorithm on same input problem and same parallel machine may or may not produce the same iterative sequence, depending on whether or not all of the processors work at the same speed in the two runs. Therefore, in a timesharing mode, the iterative sequence obtained from two different runs may be different. However, the parallel algorithm still follows the move/evaluate/decide idea followed by the sequential (two-level) simulated annealing algorithm. It tries to move from one iteration point to another, accepting a better solution, and accepting a worse solution with some probability. The parallel algorithm in [7] works the same as the sequential algorithm, but at a cost of a lot of wasted computation time. In our parallel algorithm, all of the computation provides useful information. There is no waste of computer time except the communication time if it is implemented on a loosely coupled machine.

4 Applications to the Molecular Conformation Problem

The minimization of potential energy functions of clusters of atoms is known as the molecular conformation problem. The global minima of potential energy functions are of great interests to researchers in chemistry, biology, physics, and optimization. One of the fundamental problems in molecular conformation is the minimization of the pure Lennard-Jones potential function [12]. Even this problem has been proven to be very hard. Hoare has claimed that the number of local minimizers of a cluster of n atoms grows as fast as the function $O(e^{n^2})$. Nontheless, many papers have been published on computational methods [4, 5, 11, 13, 14, 15, 18, 25, 27, 28, 29, 32, 33, 34] and putative global minima for cluster sizes as large as $n = 150$ have been reported [14, 25, 29].

The most successful algorithm for minimizing Lennard-Jones clusters has been Northby's algorithm which first finds a set of lattice local minima and then relaxes those lattice minima by continuous minimization. With this algorithm, Northby is able to publish putative global minima for cluster sizes ranging from 13 to 150 [25]. In Northby's algorithm, the lattice search part is a discrete optimization problem (actually a combinatorial one). Therefore in [22], we call this algorithm

a Discrete-Continuous algorithm. So far, the most computing intensive part in Northby's algorithm is in the discrete optimization. And the most computing intensive part in Northby's lattice search algorithm is in the search for lattice local minima where it pivots from one configuration to another with a better function value. We call each of these pivots a *move* (or just a pivot).

It should be noted that in [5, 6] general purpose global optimization algorithms have been proposed which can, without knowledge on the lattice structure, find minimizers as good as the ones reported by Northby for the Lennard-Jones clusters of size in the range $n \leq 147$, with only a few exceptions, where minimizers almost as good as the ones reported by [25] are found. To the best of our knowledge, these are the most successful applications of general purpose global optimization algorithms on the Lennard-Jones clusters.

In this paper, we apply our two-level simulated annealing algorithm to the lattice search problem, and implement the algorithm on Thinking Machines CM-5. Because of the efficient implementation of the two-level simulated annealing algorithm, we are able to get satisfactory results for the discrete minimization problem for $n = 100,000$ on the CM-5 in a relatively short time. These lattice minimizers are then relaxed to obtain ground states for the Lennard-Jones clusters. Particularly, for $n \leq 1000$, we have found lower energies than the ones reported in [22].

4.1 Lennard-Jones Potential and the IC and FC Lattices

Given n atoms (points), $p_1, p_2, \cdots, p_n$, in 3 dimensional Euclidean space, the total 2-body potential energy function is defined as

$$V_n(p) = \sum_{j=2}^{n} \sum_{i=1}^{j-1} v(||p_j - p_i||_2) \ , \qquad (1)$$

where $v(r)$ is the Lennard-Jones potential function ([12]) defined as

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

The problem is to find a configuration (positions for the n points) such that the total potential energy function $V_n(p)$ is minimized.

For each pair, the Lennard-Jones potential function $v(r) = r^{-12} - 2r^{-6}$ is plotted in Figure 4. It has only one local minimizer at $r = 1$ (which is also the global one) with function value -1. As r approaches 0, $v(r)$ approaches $+\infty$. As r approaches $+\infty$, $v(r)$ saturates to 0. Note that the function $v(r)$ is a unimodal nonconvex function.

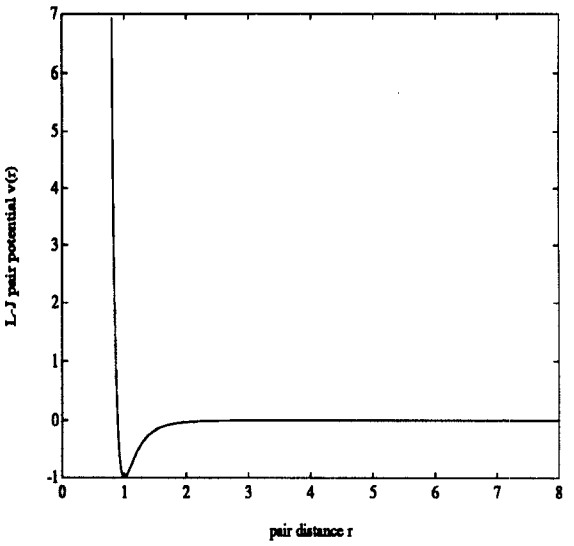

Figure 4: **Lennard-Jones pair potential function**

Finding a global minimizer of $V_n(p)$ is extremely difficult except for very small cluster sizes. The difficulty is due to the fact that while it is always possible with a supercomputer and a local minimization algorithm (e.g. quasi-Newton method) to relax any initial configuration to some local minimizer, unless the starting configuration is in the catchment basin of the global minimizer, the minimizer found may not be the global minimizer. Hoare has shown that the number of local minima in the potential energy surface of an n-atom Lennard-Jones cluster is about $O(e^{n^2})$. Thus, it is impractical to perform an undirected search for all local minima of the potential function in order to find the global minimizer, except for very small clusters.

Very often, one can better solve a problem if he/she has some physical insight into the problem. Here again, it is the case. Chemical physicists have learned from previous research that the "ground states" of Lennard-Jones clusters exhibit certain kind of lattice structures. So far, the most successful algorithms for computing ground states of Lennard-Jones clusters are based on lattice search followed by local minimization from the lattice minima, represented by the Northby algorithm [25]. As stated in [22], a critical assumption for lattice search based algorithms is that *a well-defined set of lattice structures contains at least one initial cluster configuration which relaxes to the ground state.* As described and supported by computational results in [25], the IC

and FC lattices to be described below are well-defined lattice structures for the pure Lennard-Jones clusters. We believe that in *most of the cases*, the relaxation of a global lattice minimizer will result a configuration with a lower energy than the relaxation of a non-global lattice local minimizer.

The icosahedral lattice [8, 14, 25] introduced by Mackay can be described as 20 slightly flattened tetrahedrally shaped fcc units with 12 vertices on a sphere centered at the origin. The ratio between the interatomic spacing in the 20 equilateral outer faces and the radial lines connecting the 12 vertices with the origin is $\sqrt{\frac{2}{1+\cos(\frac{\pi}{5})}}$, which is approximately 1.05146.

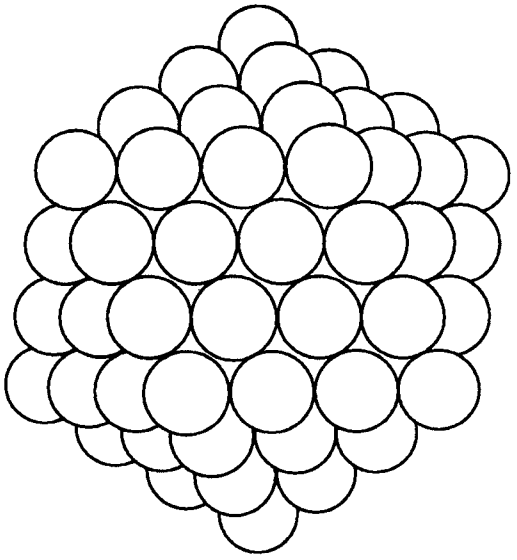

Figure 5: **An IC lattice with 147 lattice points**

For the IC lattice, the total number of lattice on each layer is 1, 12, 42, 92, $\cdots$, $10i^2+2$, $\cdots$. Therefore the number of lattice points in the sequence of closed shell IC lattice is 1, 13, 55, 147, $\cdots$, $1+(10i^3+15i^2+11i)/3$, $\cdots$.

The FC lattice consists of a smaller IC lattice enclosed by a layer of *stacking fault* icosahedral shell. This shell has 12 vertices and 20 facets as described above. However, it has fewer filling lattice points on each facet. These lattice points are located at the stacking fault positions of the IC lattice shell. The number of lattice points on the outer layer of an FC lattice is 1, 12, 32, 72, 132, $\cdots$, $10i(i-1)+12$, $\cdots$. Therefore the number of lattice points in the sequence of closed shell FC lattice is 1, 13, 45, 127, $\cdots$, $11+(10i^3+15i^2-19i)/3$, $\cdots$.

Figure 1 of [25] best describes how each of the facets are filled with other lattice points for both the IC shell and the FC shell. An IC lattice with 147 points is illustrated in Figure 5 and an FC lattice with 127 points is illustrated in Figure 6. [22] also describes how to generate these lattices.

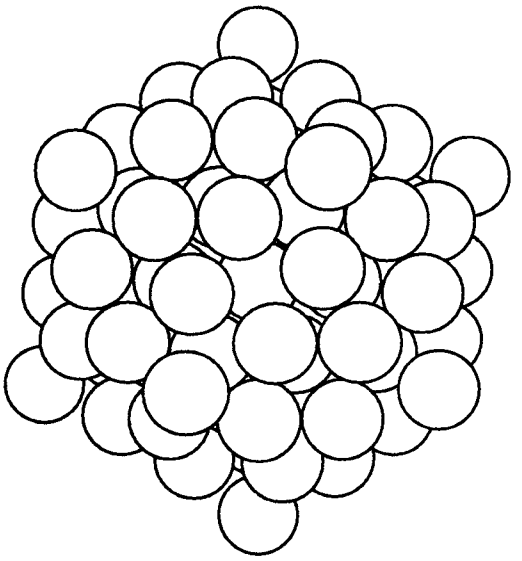

Figure 6: **An FC lattice with 127 lattice points**

4.2 Pivoting on the Lattice

In this subsection, we describe Northby's pivot algorithm for finding a lattice local minimizer.

Suppose that we want to find a lattice local minimizer of an n-atom cluster. Let us assume that we have chosen one of the two types of lattices for the lattice minimization. First, find the largest IC lattice which contains fewer than n points (if one of the IC lattices has exactly n points, we simply put all n atoms on the lattice points of that lattice and quit). Call this IC lattice the *core* and let N_{core} and I_{core} be the number of points in this IC lattice and the index set of this IC lattice, respectively. Next, find the next layer of IC (or FC) lattice which contains N_{surf} (surface) points. Let I_{surf} be its index set. If $N_{core}+N_{surf}=n$, we simply put all n atoms on the lattice points of the lattice and quit.

An initial configuration can be constructed by filling N_{core} atoms into the core lattice and randomly put the remaining $(n-N_{core})$ atoms onto the N_{surf} surface lattice sites. This is equivalent to partitioning the index set I_{surf} to two subsets I_{surf}^{filled} and I_{surf}^{vacant} such that $|I_{surf}^{filled}|=n-N_{core}$ and that site $i\in I_{surf}$ is filled with an atom if and only if $i\in I_{surf}^{filled}$.

Northby [25] computes the interaction matrix $VP(i,j)$, the pair interaction between an atom on site

i and one on site j at the very beginning of the algorithm and stores it as a lookup table. After this is done, Northby's pivot algorithm for finding a lattice local minimizer can then be summarized as follows.

Algorithm_4: Northby's Pivot Algorithm

1. {*Find the most loosely bound atom*}
   Find $i_{loose} \in I_{surf}^{filled}$ such that $i_{loose} =$

$$= arg \max_{i \in I_{surf}^{filled}} \{ \sum_{j \in I_{core}} VP(i,j) + \sum_{\substack{j \in I_{surf}^{filled} \\ j \neq i}} VP(i,j) \}. \quad (3)$$

   Site i_{loose} is called the most loosely bound filled site and the atom at that site is called the most loosely bound atom. Let $gain_{loose}$ be the maximum function value that the maximization problem in (3) achieves at i_{loose}. Apparently, this is the total contribution that the atom at site i_{loose} has towards the total potential energy.

2. {*Find the most tightly binding vacant site*}
   Find $i_{tight} \in I_{surf}^{vacant}$ such that $i_{tight} =$

$$= arg \min_{i \in I_{surf}^{vacant}} \{ \sum_{j \in I_{core}} VP(i,j) + \sum_{\substack{j \in I_{surf}^{filled} \\ j \neq i_{loose}}} VP(i,j) \}. \quad (4)$$

   Site i_{tight} is called the most tightly binding vacant site. Let $gain_{tight}$ be the minimum function value that the minimization problem in (4) achieves at i_{tight}. This is the new contribution that the atom at site i_{loose} has towards the total potential energy when moved to site i_{tight}.

3. {*Pivot on the Lattice*}
   If $gain_{tight} - gain_{loose} < 0$ then move the atom at site i_{loose} to site i_{tight} and goto step 2. Otherwise, the current configuration is a lattice local minimizer.

Figure 7: **Northby's pivot algorithm**

Moving an atom from one lattice site to another is called a *move* (or just a *pivot*) in the Northby algorithm. Each time an atom is added or removed from a site the program recalculates from VP the total potential V, and the energy change $DV(i)$ associated with adding or removing another atom at each site.

5 Lattice Search by Two-Level Simulated Annealing on the CM-5

In this section, we will describe how Northby's algorithm can be combined with our two-level simulated annealing algorithm to solve the Molecular Conformation problem on the CM-5.

Suppose that we have a cluster of n atoms. Find the largest IC lattice which contains at most n points and call this the *core* lattice. Let I_{core} be the index set of the core and define $N_{core} = |I_{core}|$. If $N_{core} = n$, put the n atoms on the core lattice and stop.

Find the next IC or FC lattice shell (depending on the lattice we are using), let I_{surf} be its index set and define $N_{surf} = |I_{surf}|$. Define $N = N_{core} + N_{surf}$ as the total number of points in the lattice. If $N = n$, put the n atoms on the N lattice points and stop.

Fill the N_{core} sites in the core with N_{core} atoms. Assign the remaining $n - N_{core}$ atoms randomly onto the surface sites. This assignment partitions the index set I_{surf} into two subsets I_{surf}^{filled} and I_{surf}^{vacant} which corresponds to the filled surface sites and the vacant surface sites, respectively.

Define the 0-1 array x with index set I_{surf} according to the above partition: $x(i) = 1$ if and only $i \in I_{surf}^{filled}$. In this way, there is a one-to-one correspondence between the lattice configurations and the 0-1 array x which has $n - N_{core}$ 1's. Define $f(x)$ to be the total potential energy function of the cluster resulted by filling N_{core} atoms in the core sites and the rest $n - N_{core}$ atoms in the surface sites determined by x. Using Northby's algorithm as the local minimization procedure, our two-level simulated annealing algorithm can then be applied to solve the combinatorial optimization problem in Molecular conformation.

The CM-5 extends TMC's existing Data Parallel programming model from Single Instruction-Multiple Data (SIMD) to Single Program-Multiple Data (SPMD). It can support both a highly synchronized Data Parallel/SIMD paradigm and a message passing paradigm which a MIMD machine would provides.

The CM-5 allows a control processor (CP) to control a large number of processing elements (PE's) by down loading to each PE an identical copy of the same program. The PE's then either execute the same code in a SIMD mode, or take different branches in that code, thus effectively emulating MIMD. Interprocessor communications are supported through two networks: the Data Network (DN) and the Control Network (CN).

The message passing library (CMMD) is used to control and coordinate program streams running on different PE's. For more detailed information about the CM-5, readers are referred to the Thinking Machines publications [30, 31].

The machine that we have used at the Army High Performance Computing Research Center/Minnesota Supercomputer Center is a 544 PE machine. The system can be partitioned into two or three partitions of either 32 and 512 PE's, or 32, 256, 256 PE's. The PE's are addressed from 0 to 31, or 255, or 511, depending on the different partitions. Each PE is a 33 MHz SPARC-2 chip with 32 MB local memory and 4 vector units. However, at the time of implementation, vector units were not supported for CMMD. Interprocessor communication has a bandwidth of 20 MB/sec within a group of 4 nearest neighbors (e.g., PE's 0, 1, 2, 3, or PE's 4, 5, 6, 7, etc.), 10 MB/sec within a group of 16 of second nearest neighbors (e.g., PE's 0-15, or PE's 16-32, etc.), and 5 MB/sec between any two PE's on the system. The machine is running under CMOST 7.1.1.

Our two-level simulated annealing algorithm has been implemented on the CM-5 in a master-slave mode. One PE (number 0 in this case) serves as the master PE, and all other PE's serve as slave PE's. The master PE is used to emulate the sheared memory assumed in the description of Algorithm_3. Each slave PE asks for a job from the master, performs a perturbation, lattice search, and decides whether to accept or reject the new solution. It then sends the computation results back to the master and asks for a new job until it is told to stop. The master PE checks incoming messages from any node. sends out new jobs to and receives computation results from the slaves, Whenever a new solution is accepted by the corresponding slave, the master also accepts that solution and makes it the new current solution. The ten (or fewer) best solutions are stored in the master node. If stopping criterion is met, it signals the slaves to stop and sends the computed results to the host.

This turns out to be very efficient both in solving the problem and in achieving a good flop rate on the machine. In particular, we have got satisfactory results for the lattice minimization problem for cluster sizes as large as $100,000$ and achieved a 0.8 giga flop/sec in double precision operations which is about one third of the theoretical peek performance of the machine as it is.

Computational results on lattice minimization are obtained on the CM-5 at the AHPCRC/MSC operated under the CMOST 7.1.1 operating system. The programs are written in F77 and employ the CMMD message passing library. We have been able to produce reasonable results for clusters with as many as 100000 atoms. Also, a rate of 818 mega flop per second is sustained on the the CM-5 with 512 PE's without vector units. Detailed computational results can be found in the more complete paper [36] and will not be presented here.

6 Conclusions

In this paper, we have developed a new kind of simulated annealing algorithm – the two-level simulated annealing algorithm for solving certain class of hard combinatorial optimization problems. A parallel version of this algorithm has also been developed. These techniques are then applied to the Molecular Conformation problem and implemented on the Thinking Machines CM-5. We have been able to get better results and get satisfactory results for much larger problems with our parallel two-level simulated annealing algorithm. We believe that our parallel two-level simulated annealing algorithm will find more and more applications in other models of Molecular Conformation problems and in hard combinatorial optimization problems from Operations Research and Computer Aided Design.

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