Lennard-Jones Energy Minimisation

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Contents

1 Introduction

The model molecular energy minimisation problem involves the geometric configuration of a cluster of atoms in two dimensions, each connected by rigid bonds of unit length, such that the total potential energy yielded by the sum of individual Lennard-Jones potentials is globally minimised. The total potential energy of the cluster is given by

$$V(r) = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left(r_{ij}^{-12} - 2r_{ij}^{-6} \right)$$

Where r is the euclidean distance between a pair of atoms and N is the number of atoms in the chain.

The energy minimisation problem is historically difficult because of the exponential relationship between the locally stable structures and the number of atoms, N, in the molecule. That is, as the size of the cluster increases, the number of local minima increases exponentially such that when N approaches 100, there exist more than 10^{140} minima [1]. It is therefore necessary to employ sophisticated search algorithms in order to make larger input sizes attainable.

Section 2 will discuss some of the research that has already taken place in this area. Section 3 will detail the algorithm proposed by this paper.

2 Literature Review

Biased modelling approaches, in which prior assumptions are made regarding the structure of optimal configurations, have been used successfully in the past to yield powerful results. Initially, for example, global minima for many of $N \leq 150$ were found using lattices derived from icosahedron [2]. However while these methods can be the most powerful, they suffer in cases when the assumed model is largely different from the real configuration [3]. Therefore, more general, less biased algorithms have been applied in order to increase robustness against such exceptional cases.

Genetic algorithms have been employed in in order to successfully extend the range of input size N that is reachable through structural optimisation [1], [4], [5]. This population based approach emulates the Darwinian process of natural selection, and works by performing crossover operations on pairs of candidate configurations over many generations until a global minimum is produced. This method has been successful in producing results that were previously unseen in literature for certain N sizes, due to its generality when compared with more biased approaches.

The Conformational Space Annealing Method is a more recent unbiased global optimisation algorithm that has produced very good results [6]. This technique is highly robust against random initial configurations thanks to its generality. As a result, it has therefore been able to produce all global minima for $n \leq 183$ without suffering from exceptional cases like those experienced by

the biased modelling algorithms. This algorithm combines concepts of Monte Carlo with Minimisation, Genetic Algorithm and simulated Annealing, and requires no specific knowledge or assumptions regarding the optimal structure. Local minimisation is performed on a set of configurations, and then similarly to the mating process of genetic algorithm, a subset of configurations is produced. A parameter D_cut is introduced and acts as a temperature variable in the annealing process. This parameter represents a distance measure between configurations and is used to maintain diversity in the population [6].

Another unbiased global optimisation algorithm, known as dynamic lattice searching (DLS), works by repeatedly constructing and searching a dynamic lattice until a global minimum is produced [3]. This lattice is built by searching the possible location sites for added atoms, which are then iteratively relocated from lattice sites of higher energy to those of lower energy. This method is very efficient because of how much it reduces the search space, but remains unbiased and therefore does not exhibit the same limitations seen in the biased modelling based techniques.

3 Proposed Optimisation Algorithm

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