



DIPARTIMENTO DI SISTEMI E INFORMATICA

New global optima for Morse clusters at $\rho = 8$
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Abstract

We recently discovered 5 new putative globally optimum configurations for Morse clusters at $\rho = 8$. This report contains some algorithmic details as well as the structures determined with our method.

Methodology

After the success obtained in solving minimum energy conformation problems for Lennard-Jones clusters (see [LS02] and [LS03]) we recently adapted our two-phase monotonic basin-hopping strategy to the minimization of Morse molecular clusters. We recall that, given two particles, the pairwise Morse interaction between them is defined as

$$v(r; \rho) = \left(e^{\rho(1-r)} - 1 \right)^2 - 1$$

where ρ is a parameter and r is the distance between the center of the two particles. A system consisting of N particles has a Morse potential given by

$$M_N(\rho) = \sum_{i=1}^N \sum_{j=i+1}^N v(\|X_i - X_j\|; \rho)$$

where X_i and X_j represent the three-dimensional coordinates of the centers of particle i and j respectively. Finding the coordinates of N particles in such a way as to globally minimize $M_N(\rho)$ for a fixed value of ρ is an extremely challenging global optimization problem which has attracted much theoretical as well as algorithmic research in the last few years. The problem becomes harder and harder as ρ increases. In <http://www-wales.ch.cam.ac.uk/~jon/structures/Morse.html> the current putative optima for $N \in [5, 80]$ are reported, with tables indicating explicitly the putative optima for $\rho = 3, 6, 10, 14$ and an indication of the range of ρ values in which those optima are believed to be optimum. In the same web site it is reported that “The location of all the global minimum at $\rho_0=3, 6, 10$ and 14 for clusters with up to 80 atoms would be a significant achievement and one which no unbiased global optimization algorithm has yet managed.”

Indeed we managed to obtain all the putative optima with a two-phase algorithm, whose details will appear elsewhere. While searching for optimum conformation at $\rho = 14$ we discovered five new conformations which, for $\rho = 8$ had an energy which is lower than the one reported in the tables. In any case these optima were obtained using a two phase algorithm in which, during what we call the first phase, a modified potential is optimized and, during the second phase, a local optimization is performed from the optimum found in the first phase. The first phase potential is a modification of the Morse one and, in the experiments whose results are displayed in this report, we used to optimize with a ρ value larger than the one used in the second phase. In particular we ran two-phase methods using $\rho = 14$ in the first phase and $\rho = 8$ in the second.

Results

Without going in much detail on the parameters used, we report here the comparison between the energy of the new structures found and the previous putative optimum reported in the Cambridge Clusters Database (CCD):

N	putative optimum	new optimum
24	-84.5623	-84.60748
25	-88.73944	-89.04075
45	-180.88844	-181.03242
48	-195.68894	-195.84211
51	-210.5258	-210.6169

Pictures 1–5 report the new and previous optimum configurations – in all the figures the structure in red on the right is the putative optimum contained in the CCD, while the structure in green on the left is the new putative optimum we discovered. It is readily seen that for $N = 24, 45, 48, 51$ the old and new structures are very similar. Indeed, once we found them, we ran our two phase non monotonic method directly using $\rho = 8$ and indeed very easily found again these structures. They are all based on icosahedral lattices and they can also be easily found with a forward procedure. [Doy03] suggests that “on going from 44B→45B→46B and 47B→48B→49B two atoms are added. If the order in which these atoms is added is reversed one gets the new structures” (the codes used here are those of the CCD). The new 24-atom structure is an icosahedron with an anti-Mackay overlayer, but with the new atom on 23A in a slightly different position to 24A. The 51-atom structure is another icosahedral structure and can be formed by adding an atom to 50B.

A slightly different analysis should be done for the new 25-atom structure, which, as can be seen from the pictures, is quite different from the previously known putative optimum. Again [Doy03] reports that “the new 25-atom structure can either be thought of as 23B (two face-sharing icosahedra) with two atoms added next to the middle of the cluster, or as three interpenetrating icosahedra with the a bent line joining the centers (for 23A it is an equilateral triangle)”. This structure appears to be a stable one for a different potential function, namely the Dzugutov potential (<http://www-wales.ch.cam.ac.uk/~jon/structures/Dzugutov/structures.html>). The fact that not only our procedure was able to improve the putative optimum for $N = 25$, but also that it discovered a Dzugutov optimum might induce to think that, with very little modification, our method should perform quite well also on Dzugutov clusters. This possibility will be explored in the future.

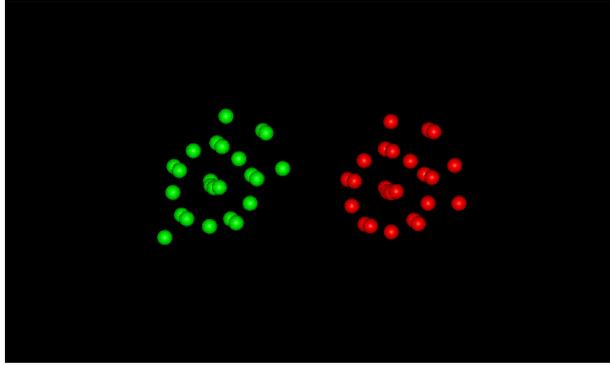


Figure 1: $N = 24$

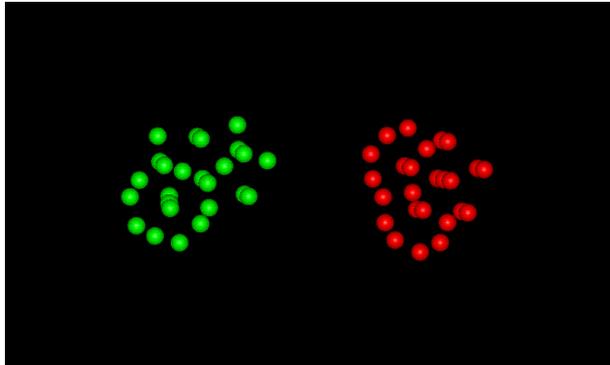


Figure 2: $N = 25$

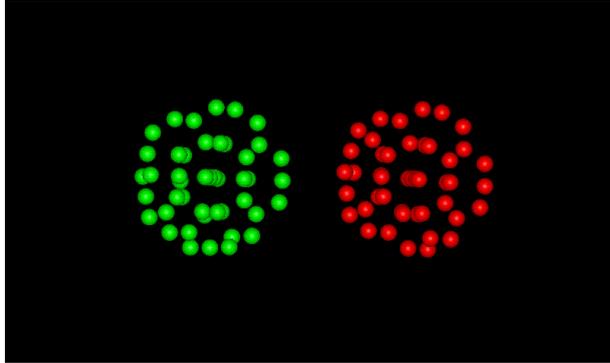


Figure 3: $N = 45$

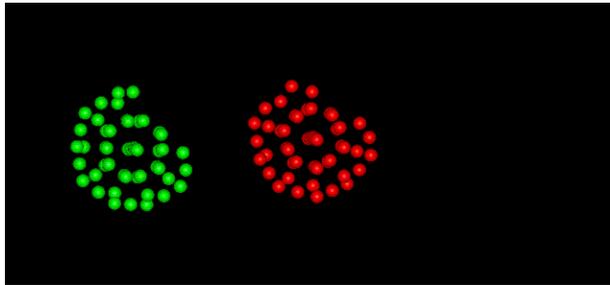


Figure 4: $N = 48$

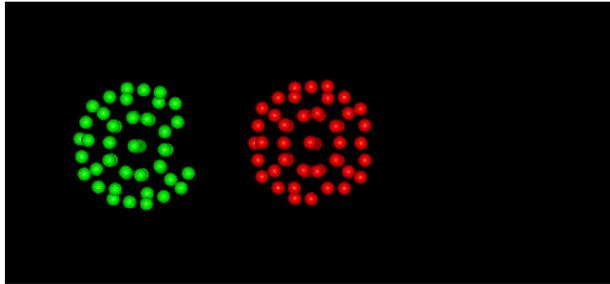


Figure 5: $N = 51$

Bibliography

- [Doy03] J.P.K. Doye. Personal communication, 2003.
- [LS02] Marco Locatelli and Fabio Schoen. Fast global optimization of difficult Lennard-Jones clusters. *Computational Optimization and Applications*, 21(1):55–70, 2002.
- [LS03] Marco Locatelli and Fabio Schoen. Efficient algorithms for large scale global optimization: Lennard-Jones clusters. *Computational Optimization and Applications (to appear)*, 2003.