Europhysics Conference on computational Physics 2004
(September, 2004, Geneva, Italy)

Basin Hopping with Occasional Jumping

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Abstract

Basin-Hopping (***BH***) or Monte-Carlo Minimization (MCM) is so far the most reliable algorithm of global optimization in chemical physics. BH transforms the complex energy landscape into a collection of basins, and explores them by hopping, which is achieved by random Monte Carlo moves and acceptance/rejection using the Metropolis criterion. In this report, we introduce the ***jumping*** process in addition to the hopping process in BH. ***Jumping is invoked when the hopping stagnates by reaching the local optima, and are achieved using the Monte Carlo move at the infinite temperature*** $T=\infty$ ***without rejection.*** *Our* ***Basin-Hopping with Occasional Jumping (BHOJ)*** algorithm is applied to the Lennard-Jones clusters of several notoriously difficult sizes N such as N=75-77, N=102-104, and N=185-187. It was found that the probability of locating the true global optima using BHOJ is significantly higher than the original BH.

Key words: ***Basin-Hopping***, ***lowest-energy structure***, ***Lennard-Jones cluster***

Ⅰ. *Structural optimization of Lennard-Jones clusters*

Minimize the Total Energy: $$E_N = \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1 \\ j\neq i}}^{N}\left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}}\right)$$

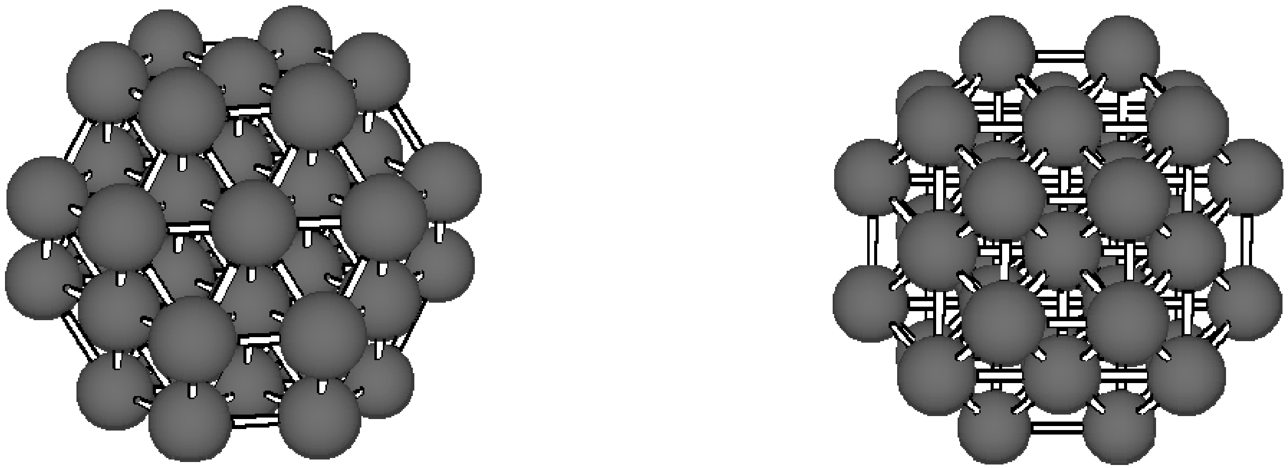

Fig 1. A example of the lowest energy structure of Lennard-Jones cluster

(38-atom LJ_{38} cluster).

Ⅱ．Basin-Hopping (BH) and Basin-Hopping with Occasional Jumping (BHOJ)

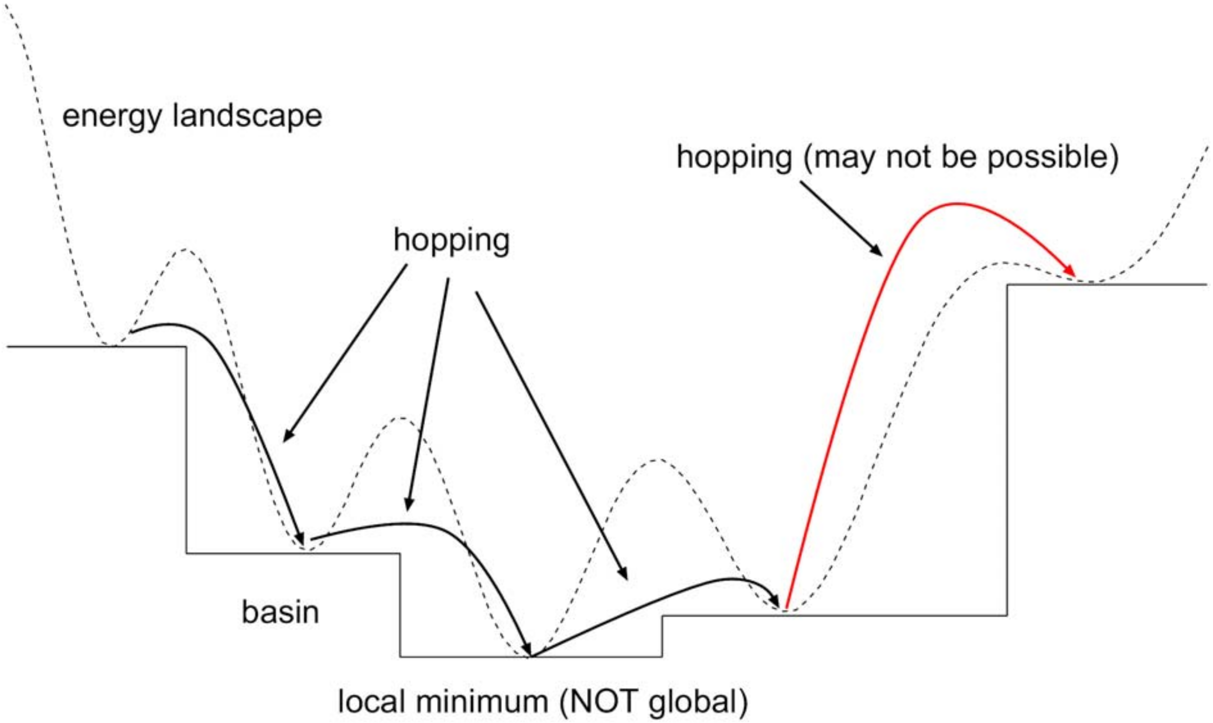

Fig 2. The Basin-Hopping (BH) algorithm.　Once the trajectory is trapped within a local minimum, it may not be able to escape from the local minimum by usual hopping.

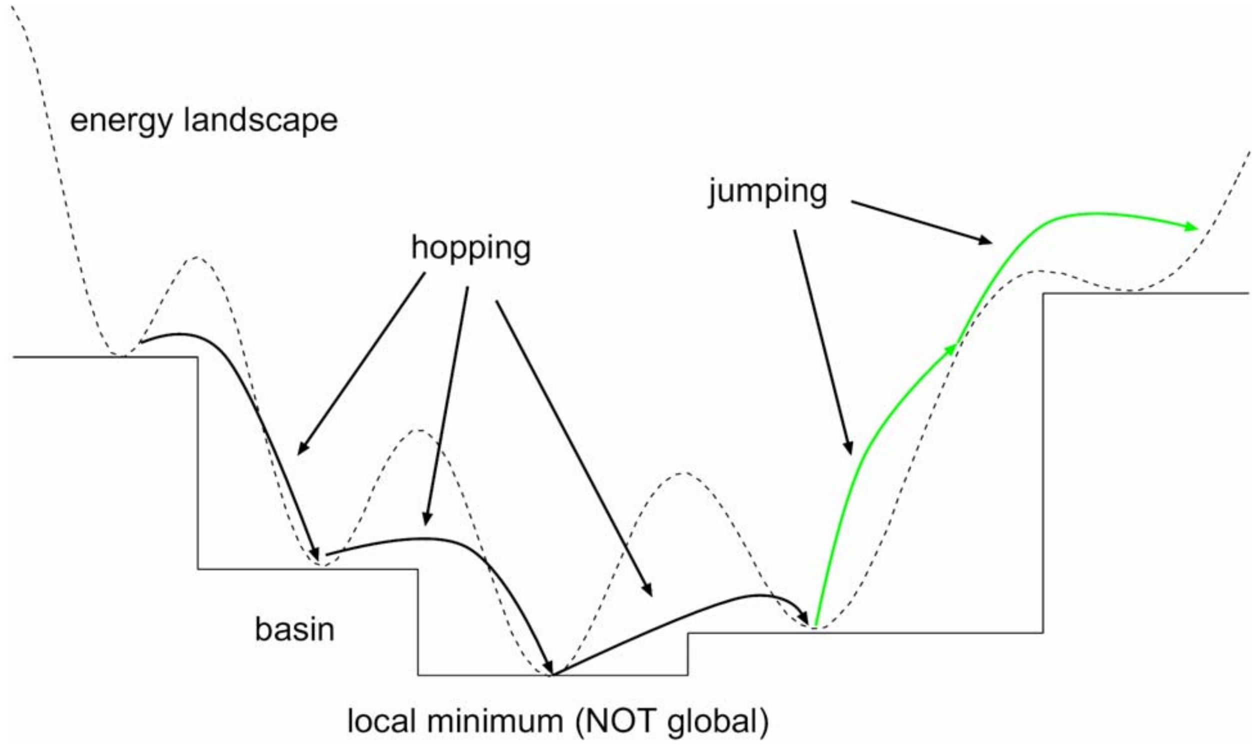

Fig 3. The Basin-Hopping with Occasional Jumping (BHOJ) algorithm. Once the trajectory is trapped within a local minimum, the jumping instead of hopping is invoked which assists the trajectory to escape from the local minimum.

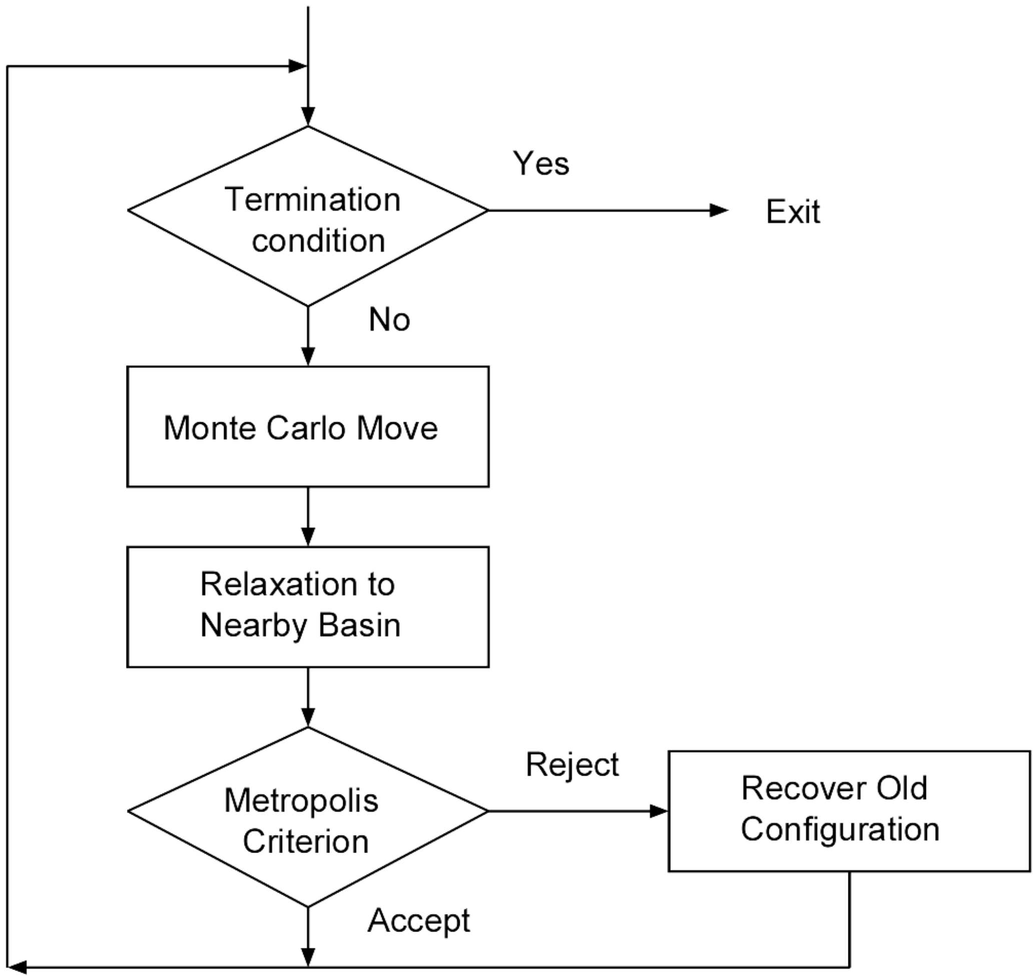

Fig 4. The flow-chart of Basin-Hopping (BH) algorithm.

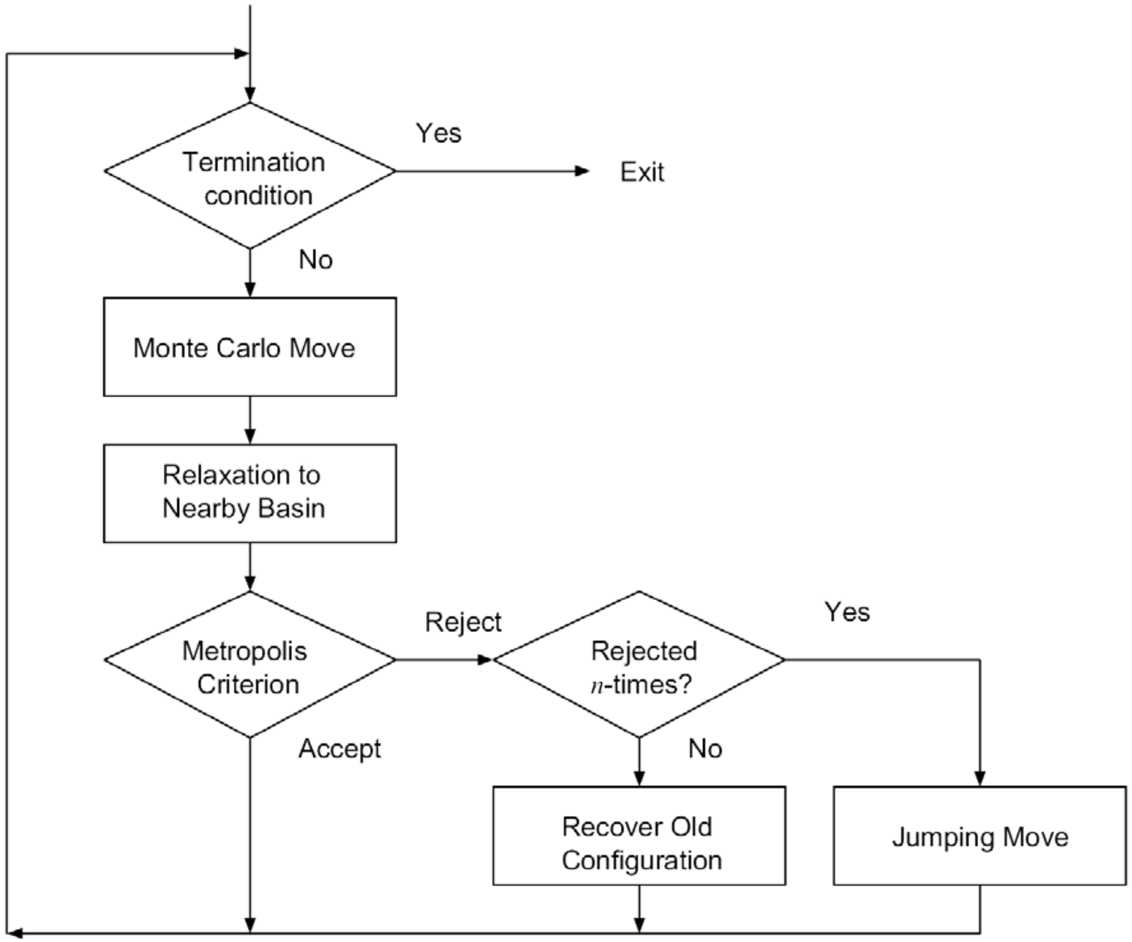

Fig 5. The flow-chart of Basin-Hopping with Occasional Jumping (BHOJ) algorithm. Maximum rejection *n* is arbitrarily fixed to *n*=10, and the jumping move consists of Monte Carlo move of 3, 5 or 7 times, which are also set arbitrarily at T=∞ without rejection.

Ⅲ. Other Optimiztion methods

1. Basin-Hopping Algorithm (BH)

   D. J. Wales & J.P.K. Doye, J. Phys. Chem. A 101 (1997) 5111.

   Pgrogam “gmin”: http://www-wales.ch.cam.ac.uk

2. Monotonic Sequence Basin-Hopping Algorithm (MSBH)

   ・ T=0 BH, Only downhill move is allowed

   R.H. Leary & J.P.K. Doye, Phys. Rev. E60 (1999) R6320

   R.H. Leary, J. Global. Opt. 18 (2000) 367

3. Parallel Fast Annealing (PFA)

   ・ Simulated Annealing + Conjugate-Gradient minimization + Parallel search

   W. Cai, H. Jiang & X. Shao, J. Chem. Inf. Comput. Sci. 42 (2002) 1099.

4. Self-Consistent Basin-to-Deformed-Basin Mapping (SCBDBM)

   ・ distance scaling method + BH

J. Pillardy, A. Liwo & H.A. Sheraga, J. Phys. Chem. A 102 (1999) 9370.

5. Genetic Algorithms

- Use biological operator instead of Monte Carlo move

D.M. Deaven et al. Chem. Phys. Lett. 256 (1996) 195

M.D. Wolf and U. Landmann, J. Phys. Chem. A 102 (1998) 6129

G. Hartke, J. Comput. Chem. 20 (1999) 1752 ETC

6. Genetic Algorithm + Lattice Search method.

- Place atoms on the icosahedral lattice (Initial Structure)

J. Northby, J. Chem. Phys. 87 (1987) 6166

D. Romero, C. Barron & S. Gomez, Comp. Phys. Commun. 123 (1999) 87.

(http://www.vcl.uh.edu/~cbarron/LJ_cluster/Ljpottable.html)

Usually these methods assume regular structure as an initial structure (Biased Search) instead of random structure (Unbiased Search).

IV. Comparison of BHOJ with other unbiased search method

Clusters	Energy	BH	MSBH	PFA	BHOJ	Jumping in BHOJ
LJ_{38}	-173.928427	87/100	124/1000	39/100	96/100	7
LJ_{75}	-397.492331	1/100	4/1000	2/200	5/100	3
LJ_{76}	-402.894866	5/100	8/1000	2/50	10/100	5
LJ_{77}	-409.083517	6/100		1/50	5/100	7
LJ_{98}	-543.665361	10/100	6/1000	4/100	10/100	3
LJ_{102}	-569.363652	3/100	31/1000	9/100	16/100	3
LJ_{103}	-575.766131	3/100		3/30	13/100	5
LJ_{104}	-582.086642	3/100		2/30	12/100	3

Tab 1. Comparison of the success rates of various unbiased searches. BHOJ shows the best performance.

V. Trajectory of the BHOJ

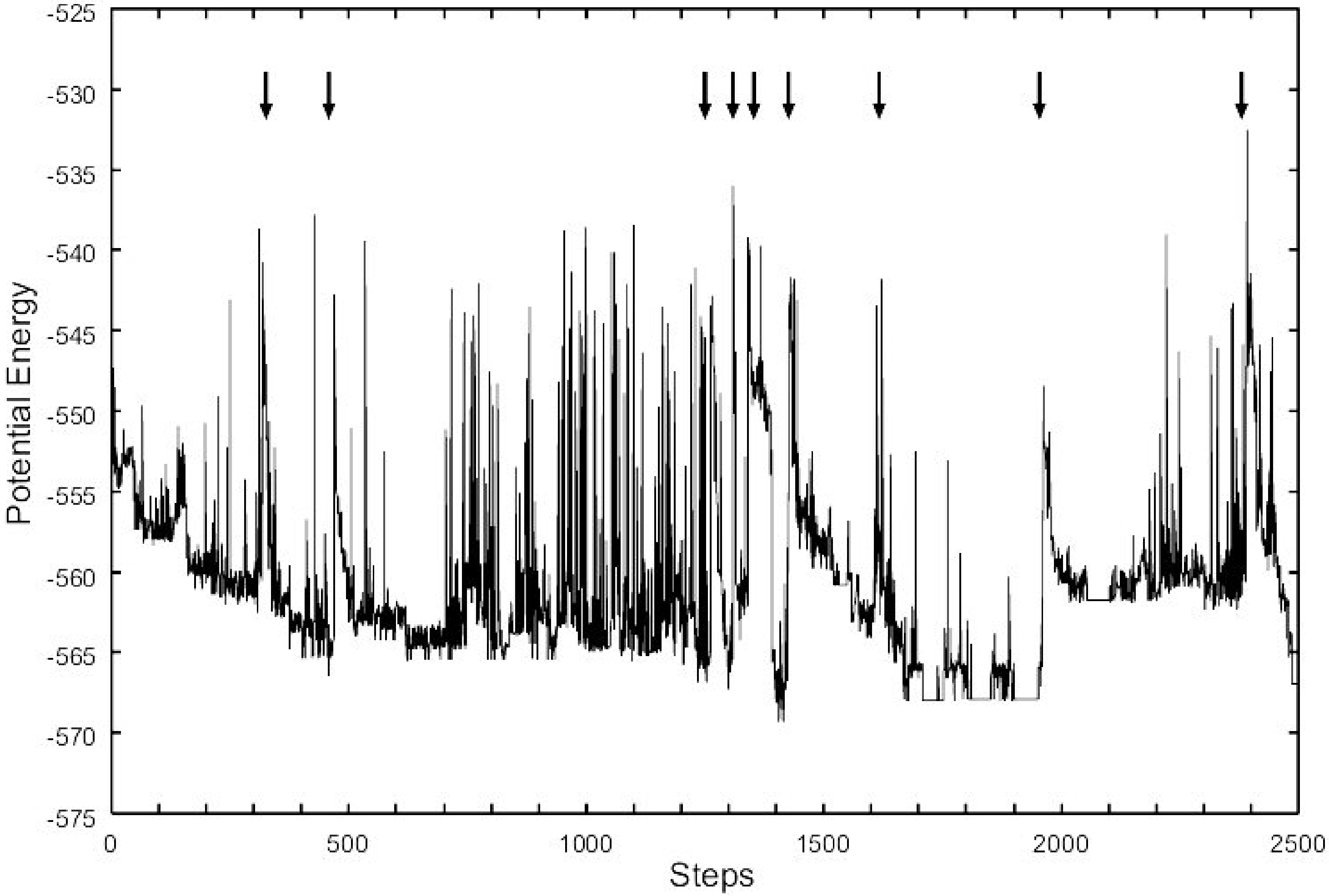

Fig. 6. A example of the trajectory of the successive run of BHOJ for LJ_{102}. Arrows indicate the times when the jumping occurs.

VI. Results for larger clusters

cluster	Energy	BH	BHOJ	Jumping in BHOJ
LJ_{107}	-602.007110	12/100	19/100	7
LJ_{185}	-1125.493794	0/500	1/500	5
LJ_{186}	-1132.669966	1/200	2/200	3
LJ_{187}	-1139.455696	0/200	2/200	3

Tab 2. A comparison of the success rates of unbiased search for larger clusters. BHOJ still seems better than original BH

VII. Conclusion

In this paper we proposed a way to improve the performance of the Basin-Hopping algorithm (BH) by introducing the jumping in addition to the hopping. We call this new algorithm as the Basin-Hopping with Occasional Jumping (BHOJ).

Experiments on benchmark problem of the Lennard-Jones clusters, in particular, for notorious difficult sizes of 75 to 77 particles $LJ_{75\text{-}77}$, of 98 particles LJ_{98}, of 102 to 104 particles $LJ_{102\text{-}104}$, and even larger 185 to 187 particles $LJ_{185\text{-}187}$ reveal that the proposed BHOJ is really superior to the original BH and other unbiased searches.

This jumping is easy to implement, and consume very little CPU resources. Any adaptive or scheduled jumping could be easily incorporated. The BHOJ with jumping will be helpful to search for the lowest-energy structures of larger clusters and more complex clusters with many body forces.

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