# Basin Hopping Algorithm

Cheyenne D. McGlothen[1]
[1]*University of Nevada, Las Vegas, Department of Physics*
*4505 S Maryland Pkwy, Las Vegas, NV 89154*
*e-mail address: cmcglothen8@gmail.com*

**Abstract:** Basin Hopping is a stochastic (a process involving a randomly determined sequence of observations) algorithm which attempts to find the global minimum of a smooth scalar function of one or more variables. For this experiment, I used the basin hopping method to determine all of the ground states for Lennard-Jones clusters for 11, 15, and 19 atoms.

## I. INTRODUCTION

Basin hopping is a global optimization framework. It is suited for hard nonlinear optimization problems with multiple variables and multimodals. It is effective for the characterization of biological macromolecules. It combines heuristic procedures with local searches to enhance its exploration of the given variable space, conducted as a series of influences followed by local optimization. The core advantage of the basin hopping method is that it moves between adjacent local minima in the variable space. This strategy is more effective when exploring high-dimensional variable spaces associated with complex physical systems, where the addition of new dimensions can result in an exponential increase in the number of minima in the space. The basin hopping method originated in the computational biology community dating back to the pioneering work of Wales, where the objective was to characterize the minima of the Lennard-Jones energy function in small atomic clusters. The term basin hopping was coined in this work. The basin hopping method is particularly suited to deal with molecular spaces, where the function sought for optimization is a complex nonconvex potential energy function summing over the interactions among atoms in a 3-dimensional molecular structure.

Optimization is the process of finding the point that minimizes a function. The objective of global optimization is to find the globally best solution of models, in the presence of multiple local optima. Formally, global optimization seeks global solution(s) of a constrained optimization model. Nonlinear models are constantly encountered in many applications, such as: in advanced engineering design, biotechnology, data analysis, environmental management, financial planning, process control, risk management, scientific modeling, and others. Their solution often requires a global search approach.

Lennard-Jones (LJ) Clusters represent a simple development of global optimization methods. They have become a much-studied test system for those global optimization methods designed for configurational problems. The minimum Lennard-Jones potential energy can be found by the N -atom cluster configuration. The LJ potential can be calculated using the following equation:

$$V_{\mathrm{LJ}} = 4\varepsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \quad (1)$$

where ε is the depth of the potential well, σ is the finite distance at which the inter-particle potential is zero, r is the distance between the particles.

## II. METHODS & RESULTS

The ground states for LJ clusters were found via Python, using the basin hopping algorithm kept within the Scipy Library. The algorithm requires three parameters: the number of iterations (or steps), the temperature (T) for the acceptance or rejection criterion, and the maximum step size (S) for use in the random displacement.

I decided to determine the ground states for LJ clusters for 11, 15, and 19 atoms. To determine those ground states, the LJ potential (1) was defined, and the total energy was calculated using an array and an initial position (Fig. 1). Then to apply the basing hopping algorithm, the code in Fig. 2 was applied. For each number of atoms, I ran the code with 50 iterations for two different values for the temperature (T) and step size (S).

The last and final step was to determine the ground state for LJ clusters for each number of atoms, in which an array was created using each value of the energy calculated using the basin hopping algorithm, and them plotted.

```
import numpy as np
from scipy.optimize import basinhopping

def LJ(r):
    r6 = r**6
    r12 = r6*r6
    return 4*(1/r12 - 1/r6)

def total_energy(positions):

    E = 0
    N_atom = int(len(positions)/3)

    for i in range(N_atom-1):
        for j in range(i+1, N_atom):
            pos1 = positions[i*3:(i+1)*3]
            pos2 = positions[j*3:(j+1)*3]
            dist = np.linalg.norm(pos1-pos2)
            E += LJ(dist)
    return E

def init_pos(N, L=5):
    return L*np.random.random_sample((N*3,))
```

Fig.1. The LJ potential was defined, and the total energy was calculated.

```
N_atom =
pos = init_pos(N_atom)
res = basinhopping(total_energy, pos, niter=, T=, stepsize=, disp=True)
```

Fig. 2. The basing hopping algorithm.

For 11 atoms (N=11)

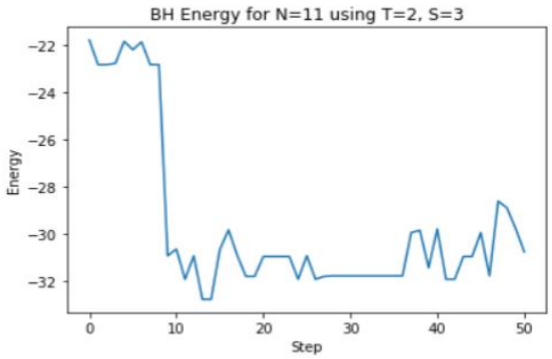


Fig. 3. BH energy for N=11, T=2, and S=3

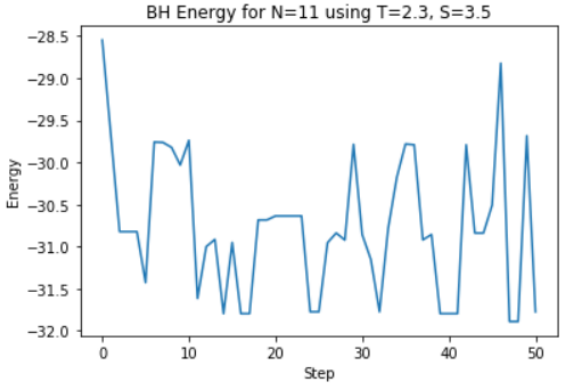


Fig. 4. BH energy for N=11, T=2.3, and S=3.5

For 15 atoms (N=15)

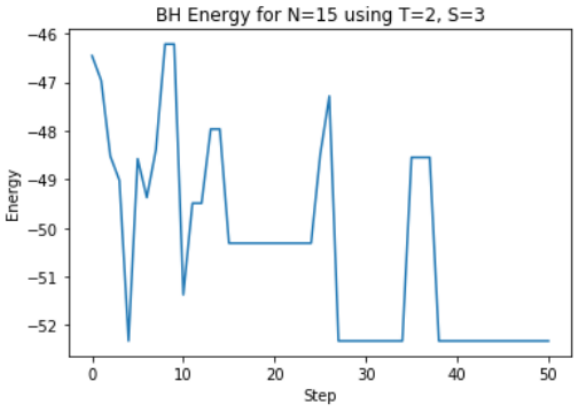


Fig. 5. BH energy for N=15, T=2, and S=3

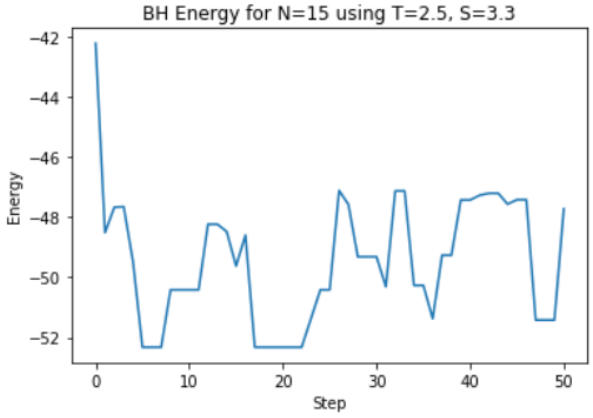


Fig. 6. BH energy for N=15, T=2.5, and S=3.3

For 19 atoms (N=19)

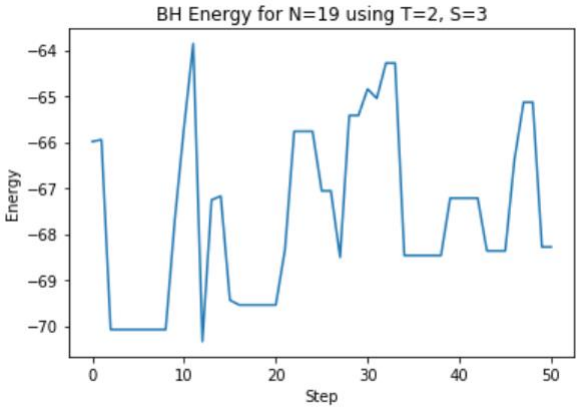


Fig. 7. BH energy for N=19, T=2, and S=3

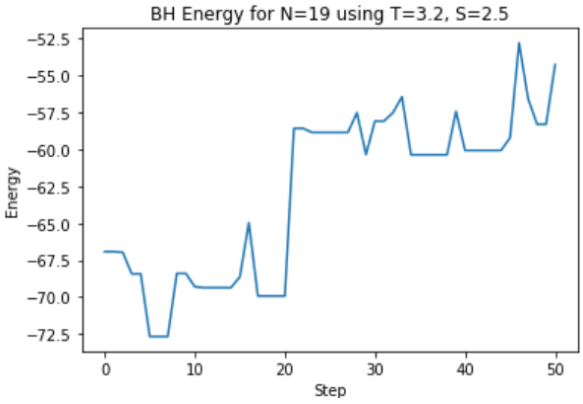


Fig. 8. BH energy for N=19, T=3.2, and S=2.5

## III. DISCUSSION & CONCLUSIONS

The application of the basin hopping algorithm is one of the most successful methods, especially for any number of atoms up to 110. It is one of the only unbiased global optimization methods which have found the global minima for some of the more complex LJ clusters.

Although the basin hopping algorithm is a simple application for determining a ground state, it can be just as simple to provide parameters that will result in a false ground state. So, when utilizing the basin hopping algorithm, you must be very calculated and careful when providing parameters so that the data will present a consistent ground state.

### A. ERROR ANALYSIS

With the exception of the data in Fig.5, each graph shows that the ground state was found, but did not consistently remain at that ground state. As you can see in my results in Fig.9, while most of my data was acurate, I could have chosen other parameters that would have improved my results.

| **Atoms** | **Basin Hopping** | **Cambridge Data** | **% Error** |
|---|---|---|---|
| 11 (T=2, S=3) | -32.766 | -32.765970 | |
| 11 (T=2.3, 3.5) | -31.8892 | -32.765970 | ~2.7% |
| 15 (T=2, S=3) | -52.3226 | -52.322627 | |
| 15 (T=2.5, S=3.3) | -52.3226 | -52.322627 | |
| 19 (T=2, S=3) | -70.338 | -72.659782 | ~ 3.3% |
| 19 (T=3.2, S=2.5) | -72.6598 | -72.659782 | |

Fig.9. Comparison of basin hopping calculations and the Cambridge dataset of the energy of LJ clusters for 11, 15, and 19 atoms.

1. https://www.hindawi.com/journals/aai/2012/674832/
2. http://mathworld.wolfram.com/GlobalOptimization.html
3. https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.basinhopping.html#scipy.optimize.basinhopping
4. https://en.wikipedia.org/wiki/Lennard-Jones_potential
5. https://scipy.github.io/devdocs/generated/scipy.optimize.basinhopping.html
6. http://doye.chem.ox.ac.uk/jon/structures/LJ/tables.150.html