# Report for basin hopping

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1. Principle and Output

(1) **Initial random configuration**: In order to record the average iteration of reaching the global optimization, I tested 25 initial random configurations(25 is enough as the result has been already closed to that of 100)

(2) **Principle determining the global minimum:** The principle I used to determine whether the program finds the global minimum is that when the relative error of the energy is smaller than 10%, the energy could be regarded as global minimum. In addition, in order to avoid extremely big iterations, we set an upper limit for the iterations which is 500000. The limit was never reached when N < 13.

(3) **Results:** The average iterations to find global optimization (N=4-13)are as follows, the whole results can be found in ***result.docx*****:**

[547.04, 730.72, 743.2, 1152.2, 1390.04, 1939.88, 2050.36, 3047.8, 14272.44, 128490.96].

(4) **Analysis:** It can noticed that the average iterations is

increasing as the N is increasing which is reasonable. In addition, there are some particular initial configurations which is capable of leading to an extremely large calculated quantity. For example, when N is 12, there are two loops having more than 100000 iterations. The reason why this condition takes place may be that the steepest descent method is quite slow for those flat parts of the potential function. And when initial configuration falls into these parts, the process becomes extremely slow.

- Parameter

  (1) **Iterations:** There are two iterations, one is the iterations of steepest descent method, the other is of the monte carlo simulation. By changing these two iterations, I found that the iterations of monte carlo simulation is more important for both accuracy of the algorithm and the speed of the calculation.

  (2) **Parameter of steepest descent:** The parameters c and t can influence the average iterations to find the global minimum, especially t. I recognized that t should be close to 1 and if it is too small or large, the process will

be slow to converge.

(3) **Rate(acceptr and newr):** The value of acceptr and newr is similar to the parameter t. I think there is no significant differences between 1.01 and 1.001 when it comes to the value of acceptr and newr. But if they are much larger, such as 1.1, the energy of global minimum will be diverging to the theoretical value.

(4) **Initial temperature and initial step_size:** these two factors strongly impact each other. When you are choosing these two factors, you have to consider both. The best combination I found for the system is step_size is 0.1 and the temperature is 0.01. The combination will have a great impact on the average iterations of the global optimization.