Energy minimum of Lennard-Jones clusters

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1 Introduction

The aim of the exercise was to find the energy minimum for a system of N points in three-dimensional space, interacting with the Lennard-Jones potential, which is expressed by the formula:

$$V(r) = 4\left(\frac{1}{r^{2a}} - \frac{1}{r^{a}}\right) \tag{1}$$

where a=6, r – distance between points.

2 Exercise description

Conjugate gradient method was used to minimize the potential. For each number N, a random distribution of points was generated, contained within a sphere of radius $1.1\sqrt{N}$. Starting from this distribution, the total potential energy was minimized and the distribution corresponding to the minimum was found. In addition, calculations were performed for various integer values of the parameter a, starting from $a = 1$ and gradually increasing the value to $a = 6$. At each stage of the calculations, the point distribution obtained for the previous value of a was used. This method allowed for obtaining more accurate results than just performing calculations for $a = 6$. The obtained results are presented in Table 1.

Table 1: The minimum energy obtained for different numbers of points, N.

N	Minimum energy	N	Minimum energy	N	Minimum energy
2	-1.0000	39	-174.8120	76	-386.8620
3	-3.0000	40	-179.7810	77	-392.7280
4	-6.0000	41	-184.8410	78	-400.3090
5	-9.1038	42	-191.3240	79	-405.4350
6	-12.7121	43	-195.8160	80	-420.7950
7	-16.5054	44	-202.5930	81	-424.8440
8	-19.7653	45	-206.4570	82	-424.3960
9	-24.1134	46	-212.4580	83	-430.3060
10	-26.7717	47	-217.8250	84	-440.8100
11	-32.7660	48	-224.2150	85	-447.3780
12	-37.9676	49	-229.0930	86	-447.1210
13	-44.3268	50	-238.3740	87	-467.1930
14	-47.8452	51	-244.4040	88	-466.0550
15	-50.1713	52	-251.3290	89	-466.2490
16	-53.9362	53	-255.5650	90	-471.3390
17	-58.1726	54	-259.5030	91	-477.9990
18	-66.5309	55	-269.5590	92	-481.5520
19	-72.6598	56	-272.3180	93	-485.1880
20	-77.1770	57	-277.2870	94	-497.6730
21	-81.6515	58	-284.9380	95	-502.4710
22	-86.8098	59	-292.6400	96	-504.8740
23	-92.8445	60	-296.1110	97	-512.0460
24	-97.3488	61	-300.0190	98	-521.7810
25	-98.1725	62	-303.8360	99	-522.6360
26	-108.3160	63	-311.6130	100	-526.7570
27	-112.8250	64	-319.0340	101	-539.2900
28	-116.0020	65	-323.6930	102	-544.0950
29	-119.1910	66	-332.0740	103	-549.3350
30	-125.2740	67	-334.5600	104	-556.1030
31	-130.3970	68	-341.8890	105	-557.4780
32	-136.6990	69	-345.1860	106	-562.7380
33	-142.4280	70	-352.4810	107	-575.8510
34	-149.0100	71	-358.1050	108	-577.1050
35	-150.9680	72	-366.9080	109	-588.2720
36	-158.9500	73	-370.4290	110	-592.6210
37	-164.4300	74	-378.7100	111	-596.2360
38	-170.6630	75	-381.4160	112	-595.4630

The duration and accuracy of the calculations depended on the parameter values used in the conjugate gradient method. These parameters are:

- k – the length of the displacement during a single iteration,
- ϵ – the value of energy gradient close to zero, at which the program terminated the iterations,
- iteration limit – maximum number of iterations for a given number of points, equal to $1000000/N$.

Increasing the iteration limit and decreasing the parameters k and ϵ allowed for obtaining more accurate results, but prolonged the computation time.
Figure 1 shows the arrangement of points corresponding to the energy minimum of -170.6630, obtained for $N = 38$. No symmetry was observed. Increasing the accuracy of the calculations should enable obtaining the expected distribution.

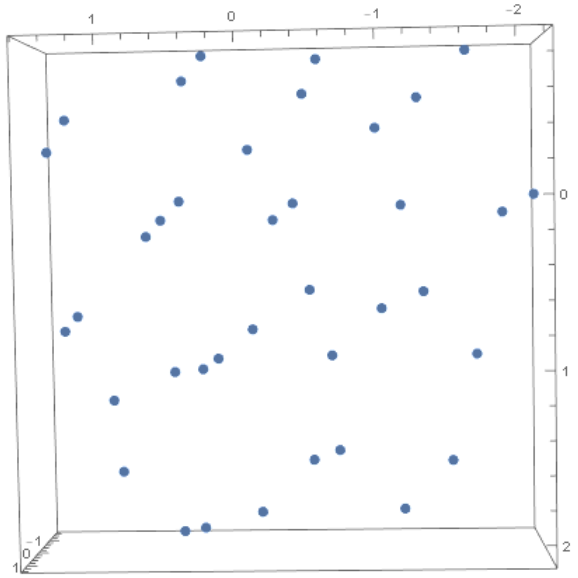

Figure 1: Arrangement of points corresponding to the minimum energy for $N = 38$.

3 Summary

The goal of the exercise was successfully achieved by finding the Lennard-Jones potential minima for distributions of N points, with N ranging from 2 to 112. Some of the obtained values differ from the expected ones, which is particularly visible for large N. It is possible to determine the minima with greater accuracy by increasing the relevant parameters of the conjugate gradient method, but this prolongs the computation time. Moreover, for a

large number of particles ($N > 37$), the total energy has a large number of local minima. Therefore, the final result significantly depends on the initial positions of the points randomly generated within the sphere of radius $1.1\sqrt{N}$. Performing multiple calculations should allow for determining the minimum with greater accuracy.

References

[1] *Expected values of energy minima*