3805ICT - Assignment 2

July, 2018

1 Background

1.1 Overview

The model molecular problem consists of N atoms connected by rigid bonds of unit length and constrained to two dimensions. The potential energy, V, of this system is given by the pairwise addition of scaled Lennard-Jones potentials. While this model problem is a very simple representation of a molecule, it is useful for developing molecular structure optimisation methods as the dimension of the problem is easily adjusted and the global minimum energy can be easily determined for any dimension.

The globally optimal conformation for the $N = 61$ molecule is shown in Figure 1.

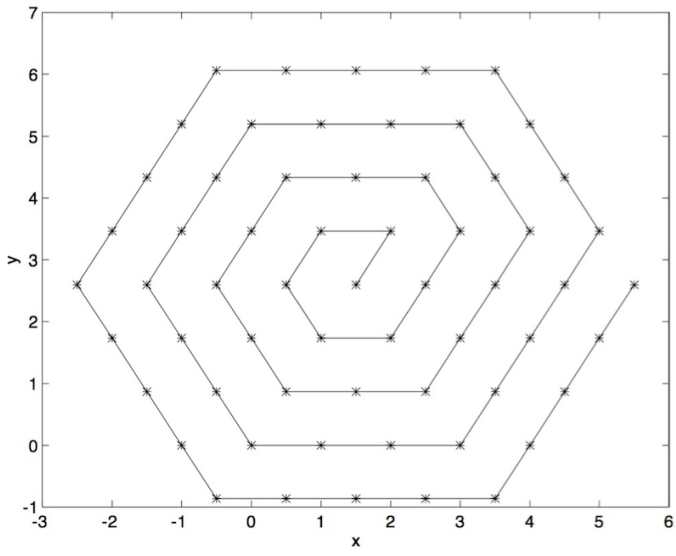

Figure 1: Globally optimal conformation for the $N = 61$ model molecular structure showing the dense hexagonal packing.

1.2 Model Encoding

The total potential energy of the system is given by

$$V = \sum_{i<j}^{N} (1/r_{ij}^{12} - 2/r_{ij}^{6})$$

where

$$r_{ij}^2 = x_{ij}^2 + y_{ij}^2$$

The use of Cartesian coordinates to specify atomic positions within a molecule during the optimisation process requires, if bond lengths and angles are assumed to remain constant, that a number of complex non-linear constraints be employed. However, if a set of internal coordinates such as bond angles in the two-dimensional case and dihedral (or torsional) angles in the three-dimensional situation are employed, then there is no requirement to specifically enforce these constraints. They arise naturally from the coordinate system.

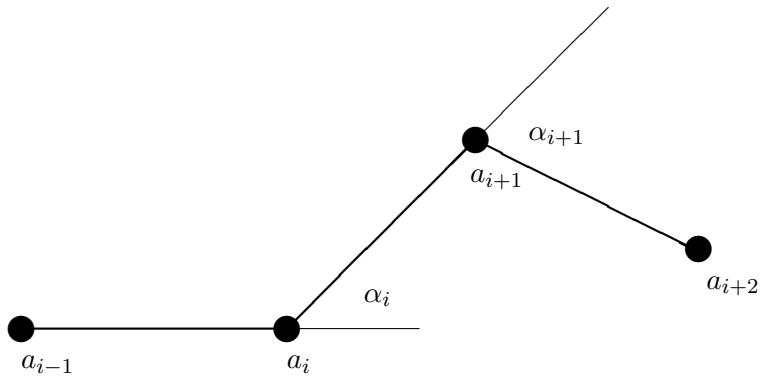

Figure 2: Bond angles (α) used to encode the model molecular structure.

With reference to Figure 2, the configuration of the model molecular structure can be encoded as a sequence of α angles in the range $-180°$ to $180°$. Clearly, and without loss of generality, one pair of atoms may be held in fixed positions. The α angles are then divided into two sets, where each set defines the configuration of the two segments of the chain which start from each of the two fixed central atoms. To implement the BFGS local optimiser (for an N atom model) we require $V_{\alpha_1}, \ldots, V_{\alpha_{N-2}}$, where α_i is as defined in Figure 2.

1.3 Results

Results are shown in Table 1 in addition to finding a final energy of -166.1 for the $N = 61$ case. All packed hexagonal energies in the range $N = 2, \ldots, 42$ and some in the range $N = 43, \ldots, 55$ were found.

N	Optimal	Found	Gen.	N	Optimal	Found	Gen.
2	-1.0	-1.0	1	29	-74.0	-74.0	5
3	-3.0	-3.0	1	30	-77.2	-77.3	18
4	-5.1	-5.0	1	31	-79.5	-79.6	1
5	-7.2	-7.2	1	32	-82.8	-82.9	9
6	-9.3	-9.3	1	33	-86.1	-86.2	10
7	-12.5	-12.5	2	34	-88.3	-88.5	5
8	-14.7	-14.7	1	35	-91.7	-91.7	9
9	-16.9	-16.9	1	36	-95.0	-95.0	36
10	-20.1	-20.1	1	37	-98.3	-98.3	31
11	-22.3	-22.3	1	38	-100.5	-100.6	17
12	-25.5	-25.6	2	39	-103.8	-103.8	23
13	-27.8	-27.8	2	40	-107.1	-107.2	23
14	-31.0	-31.0	3	41	-109.4	-109.5	6
15	-33.2	-33.2	1	42	-112.7	-112.9	8
16	-36.5	-36.5	3	43	-116.0	-115.2	50
17	-38.7	-38.8	1	44	-119.3	-119.4	48
18	-42.0	-42.1	2	45	-121.6	-121.8	39
19	-45.3	-45.3	8	46	-124.9	-125.0	22
20	-47.5	-47.5	2	47	-128.6	-127.4	50
21	-50.8	-50.8	6	48	-131.5	-130.7	50
22	-53.0	-53.0	2	49	-133.8	-133.9	6
23	-56.3	-56.4	2	50	-137.1	-137.3	30
24	-59.6	-59.6	15	51	-140.5	-139.7	50
25	-61.8	-61.9	2	52	-143.7	-142.9	50
26	-65.1	-65.1	17	53	-146.0	-146.2	20
27	-68.4	-68.5	6	54	-149.3	-148.6	50
28	-70.0	-70.7	1	55	-152.7	-150.8	50

Table 1: Packed hexagonal energies, minima and the number of generations required to achieve these minima for the model molecular structure. Optimisation was terminated when either the known global minimum was found or 50 generations had been performed.

2 Assignment

This assignment must be done individually. The submission date is as specified in the Course Profile and the submission method will be communicated during trimester.

Design an algorithm and write a program to reproduce the results shown in Table 1.

2.1 Notes

- You must actually design your own algorithm and write all program code submitted. The program must be able to be run from the command line passing the number of atoms as an argument. The naming convention for your program file is student_number_mm and try and keep the program within a single file.
- Note that as this a computationally intensive algorithm, the choice of an interpreted language such as Python is inappropriate. The best choice is C/C++ written using all possible compiler optimisations.
- You must produce a detailed paper describing your algorithms, implementation, testing and the results of the problem and performance analysis.
- You must produce a Power-point presentation summarising your algorithms, implementation, testing and the results of the problem and performance analysis.

2.2 Marking

This assignment is worth 10% of your final grade. The assignment will be marked out of 100 and marks will be allocated as follows:

- Research paper: 30 marks
- Power-point presentation: 10 marks
- Algorithmic design and implementation: 50 marks
- Quality of code (e.g. appropriate naming conventions, class / method structure, appropriate use of data structures): 10 marks

2.3 Submission

The assignment will be submitted in 3 stages as follows:

1. **Milestone 1** : Submitted by 11pm Friday of Week 3 via email as a Latex file a draft research paper with completed Introduction, Literature Review and Bibliography (10% of marks).

2. **Milestone 2** : Submitted by 11pm Friday of Week 5 via email as a Latex file a draft research paper with completed Introduction, Literature Review, Algorithm Description and Bibliography (10% of marks).

3. **Final Submission** : Submitted by 11pm Friday of Week 7 via L@G a zip file containing the complete submission (80% of marks).