

Star Coloring Problem: The DNA Solution

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Abstract— In this paper, a DNA based computing model for solving the star coloring problem is proposed. This model shows how to use DNA strands to construct solution space of molecules for the star coloring problem and how to apply the DNA algorithm to solve the star coloring problem using biological operations. The algorithm is highly parallel and has satisfactory fidelity. The time complexity of the algorithm is $O(n^2)$, where n is the number of vertices of the graph.

Index Terms— NP-complete problem, Star coloring problem, DNA based parallel algorithm, parallel computing, Polynomial time algorithm, Time complexity.

1. Introduction

Through advances in molecular biology [1, 2], it is now possible to produce 10^{18} or more DNA strands in a tube. Those 10^{18} or more DNA strands can also be applied for representing 10^{18} or more bits of information. Biological operations can be used to simultaneously operate 10^{18} or more bits of information. Or we can say that 10^{18} or more data processors can be executed in parallel. Hence, it becomes obvious that biological computing can provide a very huge parallelism for dealing with problems in the real world. Especially, the problems from the NP-complete class are well known to be exponentially more difficult than evaluating determinants whose entries are merely numerical. It is very difficult to solve these kinds of problems even if very massive supercomputers are used when the problem size becomes large.

On the other hand, DNA computers have full potential of high performance computing Technology. One test tube can be viewed as a processing unit like standard computer architecture. Furthermore, DNA

algorithms using biological operations have natural parallelism because DNA strands are separated melted, annealed) in test tubes in parallel.

Feynman [3] first proposed molecular computation in 1961, but his idea was not implemented by experiment for a few decades. In 1994 Adleman [1] succeeded to solve an instance of the Hamiltonian path problem in a test tube, just by handling DNA strands.

Lipton [4] demonstrated that the Adleman techniques could be used to solve the satisfiability problem. Adleman et al. [5] proposed sticker for enhancing the Adleman- Lipton model. In recent years methods for solving several well known NP- Complete problems [12,13,14,15,16,17,18,19,20] have been proposed.

In this paper, we develop a DNA-based algorithm to solve the star coloring problem, which is a well known NP-complete problem, based on Adleman-Lipton model. we use DNA sequence to construct a solution space for the star coloring problem. Furthermore, this work presents clear evidence of the ability of DNA based computing to solve NPcomplete problems.

The rest of the paper is organized as follows. In section 2, the Adleman-Lipton model is introduced in detail. In section 3, the star coloring problem is defined and the construction of a solution space for the star coloring problem is introduced. In section 4, a DNA algorithm is proposed to solve the star coloring problem of any undirected graph with n vertices for a given three colors. The time complexity of the proposed algorithm is described and the correctness of the algorithm is discussed. In section 5, generalized algorithm is given to solve the star coloring problem of any undirected graph with n vertices for a given l colors, where l is a positive integer.

2. The Adleman-Lipton Model

DNA is the major information storage molecule in living cells, and billions of years of evolution have tested and refined both this wonderful informational molecule and highly specialized enzymes that can either duplicate the information in DNA molecules or transmit this information to the other DNA molecules.

A DNA (deoxyribonucleic acid) is a polymer, which is strung together from monomers called deoxyribonucleotide. Distinct nucleotides are detected only with their bases. Those bases are respectively, abbreviated as A (adenine), G (guanine), C (cytosine) and T (thymine). Two single strands of DNA can form a double strand, if the respective bases are the Watson-Crick complements of each other - A matches T and C matches G; The length of the single stranded DNA is the number of nucleotides comprising the single strand. The length of the double stranded DNA is counted in the number of base pairs.

The Adleman-Lipton model: The DNA operations in the Adleman-Lipton model [1, 4, 6, 7, and 8] are described below. These operations will be used for figuring out solution of the star coloring problem.

A test tube is a set of molecules of DNA (that is a multi-set of finite strings over the alphabet A, C, G, T). Given a tube, one can perform the following operations:

1. **Denaturation:** Given a test tube T, Denaturation (T) dissociates each double strand in T into two single strands.
2. **Annealing:** Given a test tube T, Annealing (T) produces all feasible double strands in T. (The produced double strands are still stored in T after annealing).
3. **Synthesis:** Synthesis (to produce) a DNA of a desired strand.
4. **Amplification:** To make copies of the given DNA strands.
5. **Cutting:** Cut a DNA at a particular place in the strand.
6. **Ligation:** Ligate DNA strands with complementary sticky ends.
7. **Extract:** Given a tube T and a short single strand of DNA, S, the operation extract produces two tubes + (T, S) and - (T, S). + (T, S) is all of the molecules of DNA in T which contain the strand S as a sub-strand and - (T, S) is all of the molecules of DNA in T which do not contain the short strand S.
8. **Detect:** Given a tube T, the answer is 'yes' if T includes at least one DNA molecule, and the answer is 'no' if it contains none.

9. **Discard:** Given a tube T, the operation will discard the tube T.

10. **Read:** Given a tube T, the operation is used to describe a single molecule, which is contained in the tube T. Even if T contains many different molecules each encoding a different set of bases, the operation can give an explicit description of exactly one of them.

11. **Copy (T, T_i):** In parallel, this operation produces a number of copies, T_i of the set T.

12. **Union (T_i, T):** This operation in parallel creates the set T which is the set union of the sets T_i.

13. **Length-Separate:** Given a tube T and an integer n, produce the tube (T, ≤ n) consisting of all strands in T with length less than or equal to n.

3. The Star Coloring Problem

Given a graph $G = (V, E)$, where V is the set of vertices and E is the set of edges with $|V| = n$ and $|E| = m$. A proper coloring of a graph G is called the star coloring if no path of length three in G is bicolored. A proper coloring of a graph G is an assignment of colors such that no two adjacent vertices receive the same color. For a given graph G determining any assignment of 3 colors to G is a star coloring of G or not is an NP-complete problem [9].

3.1 Construction of solution of DNA sequence for the Star Coloring Problem

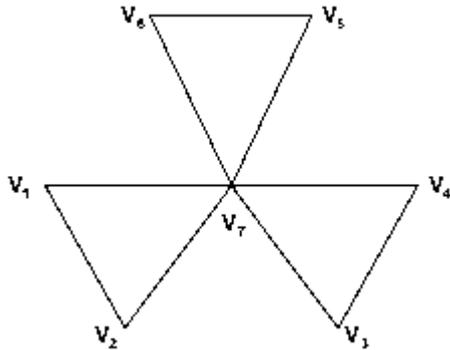
In the Adleman-Lipton model, their main idea is to first generate solution space of DNA sequences for those problems resolved. Then, basic biological operations are used to select legal solutions from the solution space. Therefore, the first step of resolving the star coloring problem is to produce a test tube which contains all possible assignment of colors to the vertices of the graph. The input is an undirected graph $G = (V, E)$, where V is the set of vertices and E is the set of edges. $|V|$ represents the number of vertices in V and $|E|$ represents the number of edges in E. Let $|V| = n$, $|E| = m$ and the three colors be c_1, c_2, c_3 .

The initial set which contains an assignment of colors to the vertices of the graph of the form $GGGN_i p_1 c_s p_1 N_i CCCGGGN_i p_2 c_s p_2 N_i CCC \dots GGGN_i p_n c_s p_n N_i CCC$, where $s = 1, 2, 3$, p_i represents the position of the vertex v_i which is a 4-mer DNA sequence, N_i is a 5-mer DNA sequence represents the i^{th} assignment of colors to the given graph where $1 \leq i \leq 3^n$. For different coding of N_i , $1 \leq i \leq 3^n$, the DNA strand $GGGN_i p_1 c_s p_1 N_i CCCGGGN_i p_2 c_s p_2 N_i CCC \dots GGGN_i p_n c_s p_n N_i CCC$ represents different assignment of colors to the given graph G. The numbers of vertices are more, use different length of oligonucleotide. An edge from a vertex v_i to v_j is encoded in two ways as $P_i^C N_i^C GGGCCCN_i^C P_j^C$ and $P_j^C N_i^C GGGCCCN_i^C P_i^C$ for

all $i = 1$ to 3^n . We encode every edge in two ways to give the effect of the undirected nature of the given graph. The edge v_i to v_j is viewed as v_i to v_j and v_j to v_i . The initial set of DNA molecules encoding all candidate solution to the star coloring problem is synthesized using ABI3948 nucleic acid synthesis and purification system [10, 11].

Illustration:

Consider the following graph.



The given graph has 7 vertices. The position of the seven vertices of the graph and colors c_1, c_2, c_3 are encoded as follows:

- P₁: ATGC
- P₂: AATG
- P₃: GCTA
- P₄: CGAA
- P₅: TTCG
- P₆: TATC
- P₇: GACT
- c₁: gtat
- c₂: gatt
- c₃: tatt

Our DNA model involves a long single strand which made of number of sub strands, and each sub strand represents the position of a vertex with an assigned color. The algorithm 1 uses three colors $c_1, c_2,$ and c_3 to color the given graph. Single strand in the form $GGGN_i p_1 c_s p_1 N_i CCC$ are used to encode one possible coloring of each vertex in the graph. The sequence N_i is used to find the i th assignment of color to the given graph. An assignment of colors to the given graph is of the form $GGGN_i p_1 c_s p_1 N_i CCCGGGN_i p_2 c_s p_2 N_i CCC \dots GGGN_i p_n c_s p_n N_i CCC$. For different coding of $N_i, i = 1$ to 3^n , this strand represents all possible encoding of the given graph. The middle sequence $CCCGGG$ is recognizable by restriction endonuclease *SmaI* which can split it at the middle site. For the above given graph, we can generate all possible assignment of colors to the given graph using the DNA codes given above. Thus, all the 3^7 DNA strands which encode the assignments of colors to the graph can be synthesized using ABI 3948 nucleic acid synthesis and purification system.

4. The DNA Algorithm for Solving the Star Coloring Problem

The proposed DNA-based algorithm to solve the star coloring problem is described in this section. It can be applied to solve the star coloring problem of any undirected graph with n vertices for a given three colors.

Algorithm.1.

1. Input (T), where the tube T, includes solution space of DNA sequences which are encoding of all possible assignments of three colors to the vertices of the given graph G.
2. For $j = 1$ to n
3. For $s = 1, 2, 3$ and all k such that $(j, k) \in E$
4. $T_1 \leftarrow + (T, p_j c_s p_j)$
5. $T_2 \leftarrow - (T, p_j c_s p_j)$
6. $T_3 \leftarrow + (T_1, p_k c_s p_k)$
7. $T_4 \leftarrow - (T_1, p_k c_s p_k)$
8. discard (T_3)
9. $T = T_2 \cup T_4$
10. EndFor
11. EndFor
12. If Detect (T) = yes then
13. Copy (T, (T', T''))
14. Add multiple copies of DNA strands GGGCCC to the test tube T', which in turn produces partial double stranded DNAs with restriction site $CCCGGG$
 $GGGCCC$
15. Add the restriction enzyme *SmaI* to the test tube T', it cuts the restriction site $CCCGGG$, giving rise to the $GGGCCC$
proper coloring of the vertices of the given graph.
16. Add DNA strands that represent the edges of the graph to the test tube T'.
17. Generate all possible walks of different length in the test tube T'.
18. $T' \leftarrow (T', = 112)$
19. If Detect (T') = yes then
20. For $1 \leq j, k, l, m \leq n, j \neq k \neq l \neq m$
21. $T' \leftarrow + (T', v_j)$
22. $T' \leftarrow + (T', v_k)$
23. $T' \leftarrow + (T', v_l)$
24. $T' \leftarrow + (T', v_m)$
25. EndFor
26. Copy (T', (U₁, U₂, U₃))
27. $U_1 \leftarrow - (U_1, c_1)$
28. $U_2 \leftarrow - (U_2, c_2)$
29. $U_3 \leftarrow - (U_3, c_3)$
30. Union ((U₁, U₂, U₃), T')
31. If Detect (T') = No then
32. Every proper coloring of the given graph G in T'' is the star coloring of the given graph G.
33. else
34. The surface is attached with the complement of $N_i, 1 \leq i \leq 3^n$, pass the content of the test tube T' through this surface. The paths of length 3 which are bicolored will attach to the complements of N_i . The sequence N_i , which are free from hybridization are separated from the surface and pour into the test

tube T'' which contains all proper coloring to the given graph G . By PCR, keep all double stranded DNA in the test tube T'' .

35. If Detect (T'') = yes
36. Proper colorings in T'' are star coloring of G .
37. else
38. Star coloring is not possible
39. else
40. Every proper coloring in T'' is a star coloring
41. else
42. No coloring is proper coloring.

4.1 Implementation of the Algorithm

This section describes the implementation of the algorithm.

- Start with all the DNA sequences that represent the assignments of colors to the given graph G .
- Eliminate all the DNA strands that do not represent the proper coloring of the graph. For each edge $(j, k) \in E$, remove the strands from a test tube T , that contain subsequences $p_j c_s p_j, p_k c_s p_k$, where $s = 1, 2, 3$.
- If the test tube T does not contain DNA strands, then conclude no coloring is a proper coloring. If not copy the content of the test tubes into two test tubes T' and T'' .
- Add multiple copies of DNA strands GGGCCC to the test tube T' , which in turn Produces partial double stranded DNAs with restriction site
- Add the restriction enzyme "SmaI" to the tube T' , it cuts the restriction site, giving rise to the proper coloring of the vertices of the given graph G .
- Add multiple copies of all the DNAs encoding the edges of the graph in the test tube T' along with the ligation enzyme. All possible walks in the given graph are generated.
- Form the tube T' , keep only the DNA strands of length 112 and discard the rest. This is done by the step $T' \leftarrow (T', =112)$. Each vertex is encoded by a DNA sequence of the form $GGGN_i P_i C_s P_i N_i CCC$. The position P_i of the vertex v_i is a 4-mer DNA sequence and N_i is a 5-mer DNA sequence and the color of the vertex is encoded by 4-mer DNA sequence. Every vertex in the graph with color is encoded by 28-mer DNA sequence. A path of length 3 contains 4 vertices. Therefore, every path of length three is encoded by $28 \times 4 = 112$ - mer DNA sequence. The step $T' \leftarrow (T', =112)$ selects all walks of length 3 for every proper coloring of the graph without any confusion. This is accomplished by gel electrophoresis technique.
- If the test tube T' contains a DNA strand then proceed to step 20. Otherwise every proper coloring in T'' is a star coloring.

- Checking the distinctness of the vertices of the walks obtained in steps 20-25: produce multiple copies of complement of the vertex v_1 and pour into a test tube T' , complement of v_1 anneal to the vertex v_1 . In a test tube T' , we have three different types of DNA strands. The vertex v_1 either occur twice or once or no occurrence in the DNA strands. Remove all DNA strands in which v_1 occurs twice using gradient centrifugation process. Denature all the remaining strands in the test tube T' to get the single stranded DNA. Repeat this process to all the remaining vertices. After completing this process the test tube T' contains all paths of length 3.

- Copy the content of the test tube T' into three test tubes U_1, U_2, U_3 . The test tube U_1 retains all the DNA strands that do not contain c_1 as a substring, the test tube U_2 retains all the DNA strands that do not contain c_2 as a substring, and the test tube U_3 retains all the DNA strands that do not contain c_3 as a substring. This step can be accomplished by the operation separation.

- Pour the content of the test tubes U_1, U_2, U_3 into a single test tube T' . If the test tube T' does not contain a DNA strand every proper coloring of the given graph G is a star coloring of G . Otherwise the surface is attached with the complement of $N_i, 1 \leq i \leq 3^n$, pass the content of the test tube T' through this surface. The paths of length 3 which are bicolored will attach to the complements of N_i . The sequences N_i , which are free from hybridization are separated from the surface and pour into the test tube T'' which contains all proper coloring to the given graph G . By PCR, keep all double stranded DNA in the test tube T'' . If Detect (T'') = yes, then the proper colorings in T'' are star coloring of G . Otherwise star coloring is not possible.

4.2 The Complexity of the DNA Algorithm

The star coloring problem with three colors for any undirected n -vertex graph G can be solved with $O(n^2)$ biological operations in the Adleman-Lipton model.

The algorithm described in section 4 can be applied for solving the star coloring problem for any undirected n -vertex graph G with given three colors. This Algorithm includes three main steps. The steps 2-11 are mainly used to determine the proper coloring of G and to remove illegal coloring of G from all of the $3n$ possible assignment of colors to the given graph G . The steps 20-25 select all paths of length 3. The steps 26-30 are used to check the bicoloredness of the path of length 3. For each vertex $v_i \in V, 1 \leq i \leq n$ and the three colors c_1, c_2, c_3 , the steps 4 and 5 take $3n$ extraction operations. Since every vertex $v_i \in V$, has at most $n-1$ adjacent vertices, the steps 6 and 7 take $3n \times 3(n-1)$ extraction operations. The step 8 takes $3n$ discard operations. The steps 12-19 take one step each to perform cutting the restriction site, adding DNA strands that represent the edges of the graph and to generate all possible walks. The steps 20-25

need $4n$ biological operations to detect the path of length 3. The steps 26 and 30 take one step each to copy and union of the content of the DNA strands. The steps 27, 28 and 29 take one step each to detect the DNA strands in which only two colors are used. The steps 31 and 35 take one step each to detect the content of the test tube. Hence, the time complexity of Algorithm is $O(n^2)$ biological operations in the Adleman-Lipton model.

4.3 Correctness of the Algorithm

The star coloring problem with three colors for any n -vertex undirected graph can be resolved using the algorithm proposed in section 4.

The input of the algorithm is a test tube, which contains all $3n$ possible assignment of colors to the given n -vertex undirected graph G .

First the algorithm detects all possible proper coloring of G by repeating the steps 2 to 11 for n number of times. The first test tube T_1 contains all the DNA strands in which the first vertex v_1 has the color c_1 , the second test tube T_2 contains all the DNA strands in which the first vertex v_1 has the color c_2 or c_3 . The third test tube T_3 contains all the DNA strands in which the vertex v_1 and its adjacent vertices have the color c_1 . The fourth test tube T_4 contains all the strands in which the vertices adjacent to the vertex v_1 have the colors c_2 or c_3 . Therefore the test tube T_3 collects all the strands in which the vertices adjacent to v_1 and the vertex v_1 have the same color and the test tube T_4 collects all the strands in which the vertices adjacent to v_1 and the vertex v_1 have different colors. Step 8 uses the “discard operation” to remove all the illegal coloring to the vertex v_1 and its adjacent vertices for the color c_1 . Step 9 merges the content of the tubes T_2 and T_4 . Now the test tube T contains the DNA strands in which the first vertex v_1 has the color c_2 or c_3 and the DNA strands in which the first vertex v_1 has the color c_1 and its adjacent vertices have different colors c_2 or c_3 . By repeating the same procedure for the vertex v_1 with the remaining two colors c_2 and c_3 , the test tube T contains all the DNA strands in which the vertex v_1 and its adjacent vertices have different colors. The steps 2-11 are repeated for all the remaining $n-1$ vertices. If the test tube T does not contain a DNA strand, no coloring is a proper coloring otherwise copy the content of the test tube T into two test tubes T' and T'' . Add multiple copies of DNA strands GGGCCC to the test tube T' , which in turn produces partial double stranded DNAs with restriction site. Now, the algorithm checks the star coloring for each proper coloring of the given graph G . Add the restriction enzyme “SmaI” to the tube T' , which in turn cuts the restriction site, giving rise to the coloring of the vertices of the graph. Add DNA strands that represent the edges of the graph to the tube T' . By ligation reaction all the walks of different length are generated in the tube T' . In coding, the 3^n assignment of colors to the graph is distinguished by the sequence N_i , the edges are encoded with all the sequences N_i , $1 \leq i \leq 3^n$, by ligation reaction all walks are generated for different assignment of colors without confusion.

Next the test tube T' retains all the DNA strands of length 112 (that is a walk of length 3). If the test tube T' contains no strand then every proper coloring in T'' is a star coloring. Otherwise, the steps 20-25 are used to find all the paths of length 3. Now the test tube T' contains all the path of length 3. Copy the content of T' into three test tubes U_1 , U_2 and U_3 . The test tube U_1 collects all the strands which have the colors c_2 and c_3 . The test tube U_2 collects all the strands which have the colors c_3 and c_1 . The test tube U_3 collects all the strands which have the colors c_1 and c_2 . The step 30 uses “union operation” to merge the contents of the test tubes U_1 , U_2 and U_3 into one test tube T' . If the test tube T' does not contain a DNA strand every proper coloring of the given graph G is a star coloring of G . Otherwise the surface is attached with the complement of N_i , $1 \leq i \leq 3^n$, pass the content of the test tube T' through this surface. The paths of length 3 which are bicolored will attach to the complements of N_i . The sequences N_i , which are free from hybridization are separated from the surface and pour into the test tube T'' which contains all proper coloring to the given graph G . By PCR, keep all double stranded DNA in the test tube T'' . If Detect (T'') = yes, then the proper colorings in T'' are star coloring of G . Otherwise star coloring is not possible.

5. The DNA Algorithm for Solving the Star Coloring Problem with l Colors

We can extend Algorithm1 to solve the star coloring problem with l colors. The following DNA algorithm is proposed to solve the star coloring problem of any undirected graph with n vertices for a given l colors, where l is a positive integer.

Algorithm.2.

1. Input (T), where tube T , includes solution space of DNA sequences to encode all l^n possible assignment of colors to the vertices of the given graph G .
2. For $j = 1$ to n
3. For $s = 1, 2, 3, \dots, l$ and all k such that $(j, k) \in E$
4. $T_1 \leftarrow + (T, p_j c_s p_j)$
5. $T_2 \leftarrow - (T, p_j c_s p_j)$
6. $T_3 \leftarrow + (T_1, p_k c_s p_k)$
7. $T_4 \leftarrow - (T_1, p_k c_s p_k)$
8. discard (T_3)
9. $T = T_2 \cup T_4$
10. EndFor
11. EndFor
12. If Detect (T) = yes then
13. Copy ($T, (T', T'')$)
14. Add multiple copies of DNA strands GGGCCC to the test tube T' , which in turn produces partial double stranded DNAs with restriction site $CCCGGG$
GGGCCC
15. Add the restriction enzyme SmaI to the test tube T' , it cuts the restriction site $CCCGGG$, giving rise to the
GGGCCC
proper coloring of the vertices of the given graph.

16. Add DNA strands that represent the edges of the graph to the test tube T' .
17. Generate all possible walks of different length in the test tube T' .
18. $T' \leftarrow (T', =112)$
19. If Detect (T') = yes then
20. For $1 \leq j, k, l, m \leq n, j \neq k \neq l \neq m$
21. $T' \leftarrow + (T', v_j)$
22. $T' \leftarrow + (T', v_k)$
23. $T' \leftarrow + (T', v_l)$
24. $T' \leftarrow + (T', v_m)$
25. EndFor
26. For $r = 1$ to l
27. For $s \neq r, 1 \leq s \leq l$
28. $T' \leftarrow + (T', c_r)$
29. $T' \leftarrow + (T', c_s)$
30. For $t = 1$ to $l, t \neq r, s$
31. $T' \leftarrow + (T', c_t)$
32. EndFor
33. EndFor
34. EndFor
35. If Detect (T') = No then
36. every proper coloring of the given graph G in T'' is the star coloring of the given graph G .
37. else
38. The surface is attached with the complement of $N_i, 1 \leq i \leq 3^n$, pass the content of the test tube T' through this surface. The paths of length 3 which are bicolored will attach to the complements of N_i . The sequence N_i , which are free from hybridization are separated from the surface and pour into the test tube T'' which contains all proper coloring to the given graph G . By PCR, keep all double stranded DNA in the test tube T'' .
39. If Detect (T'') = yes
40. Proper colorings in T'' are star coloring of G .
41. else
42. Star coloring is not possible
43. else
44. Every proper coloring in T'' is a star coloring
45. else
46. No coloring is proper coloring.

6. Conclusion

DNA computing is a computational paradigm that provides advantages over conventional electronic computing techniques. 1 μmol of DNA in 1 liter of water contains about 10^{18} strands. If we consider every strand as a processor and that operations takes several minutes, 1000s, then such a DNA based computing would execute 10^{15} operations per second. If the ligation of two DNA molecules is considered as a single operation, the number of operations per second during the ligation step would exceed that of current super computer by more than thousand fold. The major advantage of DNA computing lies in its high parallelism.

In this paper, we present DNA based algorithm for solving star coloring problem based on biological operations in Adleman-Lipton model. Our algorithm can

determine not only the star coloring but also all the star coloring of the given graph in polynomial time. The efficiency of our method can be seen from the time complexity of our algorithm $O(n^2)$.

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