FULLERENE NANODISCS: FROM CHEMISTRY TO COMBINATORICS

WPCCG 2021
Workshop de Pesquisa em Computação dos Campos Gerais

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4º Workshop de Pesquisa em Computação dos Campos Gerais (WPCCG 2021)

Engenharia de Sistemas e Computação PESC/Coppe 50 Anos 1970 - 2020

1. Fullerene Graphs

1.1 Fullerene: A graph class modeling a molecule

In 1985 a new carbon allotrope was reported in the scientific community: C_{60}. A group of scientists, led by Englishman Harold Walter Kroto and Americans Richard Errett Smalley and Robert Curl, trying to understand the mechanisms for building long carbon chains observed in interstellar space, discovered a highly symmetrical, stable molecule, composed of 60 carbon atoms different from all the other carbon allotropes.

The C_{60} has a structure similar to a soccer hollow ball (Figure 1), with 32 faces, being 20 hexagonal and 12 pentagonal. They decided to name the C_{60} *buckminsterfullerene*, in honor of American architect Richard Buckminster Fuller, famous for his geodesic dome constructions, which were composed of hexagonal and pentagonal faces.

At the end of the 1980s, other carbon allotrope molecules with similar spatial structure to the C_{60} were reported called fullerene molecules [1].

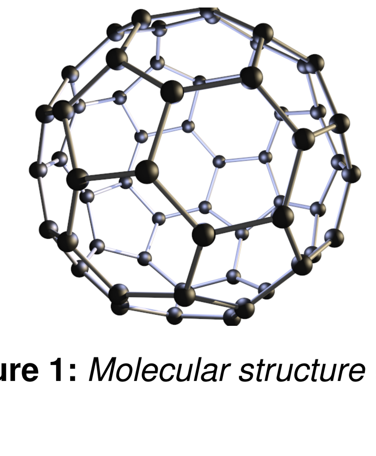

Figure 1: *Molecular structure of C_{60}.*

The buckminsterfullerene was the first new allotropic form discovered in the 20th century, and earned Kroto, Curl and Smalley the Nobel Prize in Chemistry in 1996. Nowadays fullerene molecules are widely studied by different branches of science, from medicine to mathematics. These molecules are supposed to contribute to transport chemotherapy, antibiotics or antioxidant agents and released in contact with deficient cells.

1.2 Fullerene Graphs

Each fullerene molecule can be described as a planar graph in which the atoms and the bonds are represented by the vertices and edges of the graph, respectively, preserving the geometric properties of the original fullerene molecule. Thus, we define a fullerene graph as cubic, planar, 3-connected graph whose faces are pentagonal or hexagonal (Figure 2).

The famous Euler's formula for connected planar graphs $n + f - m = 2$ relates the number f of faces, the number m of edges and the number n of vertices, and implies that every fullerene graph must contain exactly 12 pentagons, and that the smallest fullerene graph is the well known dodecahedron with 20 vertices where all faces are pentagons [2].

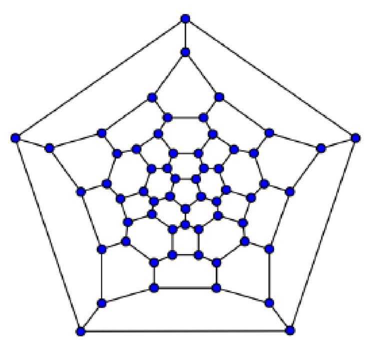

Figure 2: *Fullerene graph of C_{60}.*

1.3 Fullerene Nanodiscs

The fullerene nanodiscs, or nanodiscs D_r of radius $r \geq 2$, are structures composed of two identical flat covers connected by a strip along their borders. While in the nanodisc covers there are only hexagonal faces, in the connecting strip, besides the hexagonal faces, additional 12 pentagonal faces are arranged. Please refer to Figure 3 where the smallest fullerene nanodisc graphs are depicted. In each fullerene nanodisc graph, we highlight in the connecting strip the 12 pentagons.

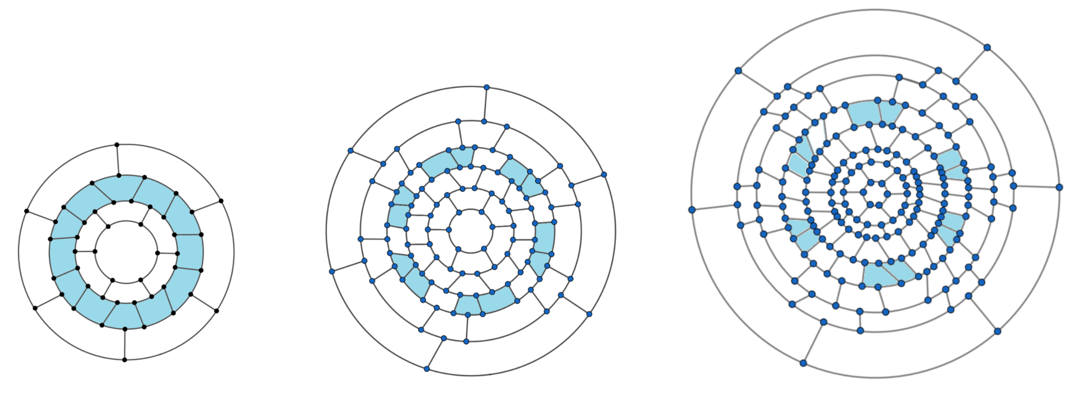

Figure 3: *The smallest fullerene nanodisc graphs.*

A nanodisc graph of radius $r \geq 2$, denoted by D_r, has its faces arranged into layers, one layer next the nearest previous layer starting from an hexagonal cover until we reach the other hexagonal cover [2]. The sequence $\{1, 6, 12, \ldots, 6(r-1), 6r, 6(r-1), \ldots, 12, 6, 1\}$ provides the amount of faces on each layer of the nanodisc graph D_r. Note that there is an odd number of $2r+1$ layers, and we call the layer with $6r$ faces the central layer. For D_2 the layer sequence is $\{1, 6, 12, 6, 1\}$, for D_3 is $\{1, 6, 12, 18, 12, 6, 1\}$ and for D_4 is $\{1, 6, 12, 18, 24, 18, 12, 6, 1\}$ (see Figure 3). The auxiliary cycle sequence provides the sizes of the auxiliary cycles that define the layers $\{C_6, C_{18}, \ldots, C_{12r-6}, C_{12r-6}, \ldots, C_{18}, C_6\}$. For example, for D_2 the cycle sequence is $\{C_6, C_{18}, C_{18}, C_6\}$, for D_3 is $\{C_6, C_{18}, C_{30}, C_{30}, C_{18}, C_6\}$, and for D_4 is $\{C_6, C_{18}, C_{30}, C_{42}, C_{42}, C_{30}, C_{18}, C_6\}$ (see Figure 3). A nanodisc graph D_r contains $12r \times r$ vertices and $18r \times r$ edges.

2. Combinatorial Results

The 12 pentagonal faces are distributed in the central layer among its $6r$ faces with the other $(6r - 12)$ hexagonal faces. This is the key property of fullerene nanodiscs [2]. Note that the central layer is defined by two auxiliary cycles, each of size $12r - 6$. The 5 vertices of each pentagon are partitioned such that 3 vertices appear consecutively in one cycle and 2 vertices appear consecutively in the other cycle. We say that two pentagons in the central layer are partitioned in the same way if each pentagon has 3 vertices in the same cycle C_{12r-6}. For $r \geq 2$, in a D_r, we may have choice to distribute and to partition the 12 pentagonal faces.

Lemma 1
A nanodisc D_r, $r \geq 2$, cannot have two consecutive pentagons in the central layer partitioned in the same way.

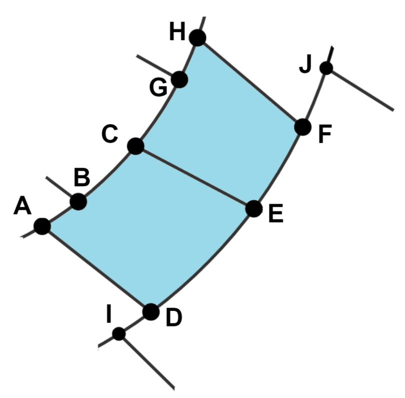

Figure 4: *Two consecutive pentagons partitioned in the same way.*

Observe that there are two ways of partitioning a hexagon in a layer defined by auxiliary cycles C and C'. We may place 3 vertices of the hexagon in each auxiliary cycle to obtain a balanced hexagon, or we may place 4 vertices of the hexagon in one auxiliary cycle say C and the other 2 vertices are placed in C' to obtain an unbalanced hexagon. The following results are obtained through the rigidity of the construction of the layers of a nanodisc.

Lemma 2
Consider the fullerene nanodisc D_r, $r \geq 2$, and its layers consisting of 6 hexagons. All the hexagons in these layers are unbalanced.

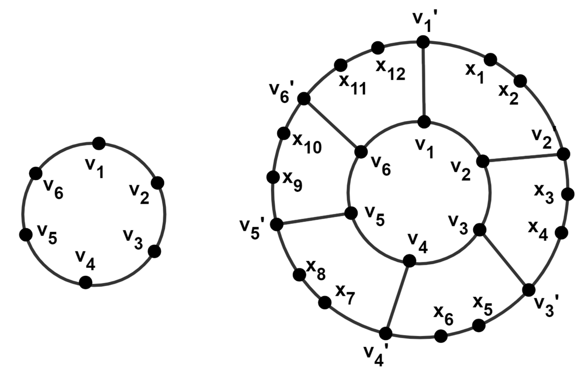

Figure 5: *Construction of layer consisting of 6 hexagons in a fullerene nanodisc D_r, $r \geq 2$.*

Theorem 1. Lemmas 1 and 2 ensure that D_2 shown in Figure 3 is unique.

Lemma 3
In D_r, $r \geq 3$, the layers consisting of 12 hexagons cannot have two consecutive hexagons partitioned in the same way.

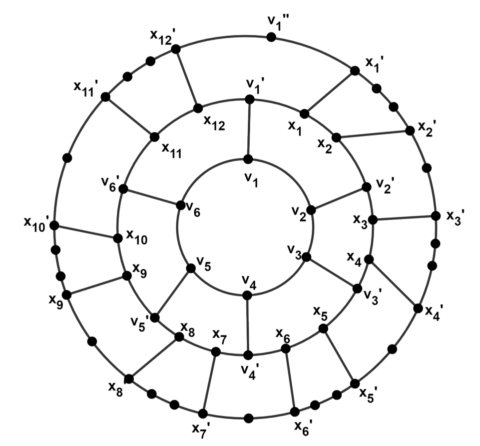

Figure 6: *Construction of layer consisting of 12 hexagons in a fullerene nanodisc D_r, $r \geq 3$.*

Lemma 4
The fullerene nanodisc D_r, $r \geq 3$, cannot have three consecutive pentagons in the central layer.

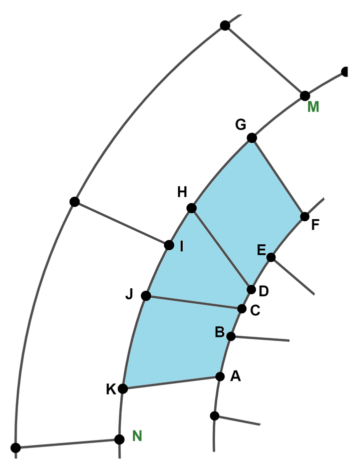

Figure 7: *Three pentagons arranged alternately in the central layer of D_r.*

In the central layer of D_3, we have 12 pentagons distributed among 6 hexagons. By Lemma 1, we cannot have two consecutive pentagons partitioned in the same way. By Lemma 4, we cannot have three consecutive pentagons. So, among the 6 hexagons, the 12 pentagons must appear in pairs of consecutive pentagons where each pair is not partitioned in the same way.

Theorem 2. Lemmas 1, 3 and 4 ensure that D_3 shown in Figure 3 is unique.

Lemma 5
Consider the fullerene nanodisc D_r, $r \geq 4$, and its layers containing 18 hexagons. Between each pair of unbalanced hexagons, there is a pair of consecutive balanced hexagons.

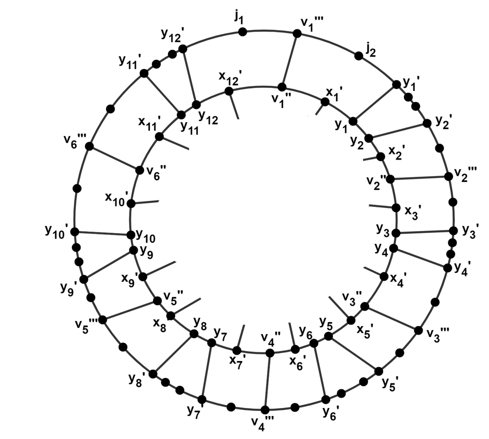

Figure 8: *Construction of layer consisting of 18 hexagons in a fullerene nanodisc D_r, $r \geq 4$.*

In the central layer of D_4, we have 12 pentagons distributed among 12 hexagons. By Lemma 1, we cannot have two consecutive pentagons partitioned in the same way. By Lemma 5, we cannot have three consecutive pentagons. So, we have two forms to distribute the pentagons and the hexagons:

- The pentagons and the hexagons are distributed alternatingly;
- Among the 12 hexagons, the 12 pentagons in pairs of two consecutive pentagons such that each pair is not partitioned in the same way.

Theorem 3. The two non isomorphic nanodiscs D_4 are shown in Figure 9.

In order to describe the number of non isomorphic nanodiscs D_r, we introduce an auxiliary t parameter, $0 \leq t \leq r - 1$, defined as the number of hexagons arranged between the pentagons in the central layer, and denote the nanodisc by $D_{r,t}$ (see Figure 9).

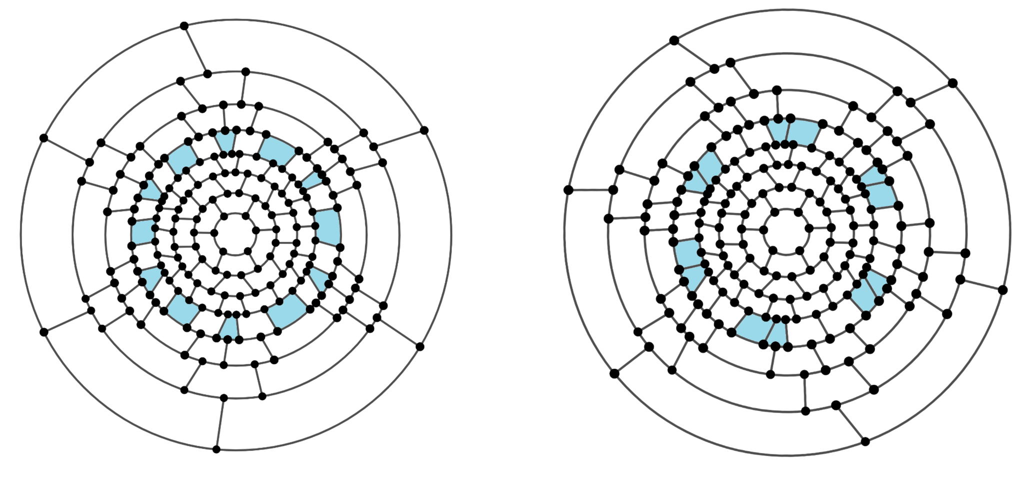

Figure 9: *The two non isomorphic fullerene nanodiscs D_4.*

References

[1] KROTO, H. et al; *C_{60}: Buckminsterfullerene* Nature, 1985.

[2] NICODEMOS, D. de S. *Diâmetro de Grafos fulerenos e Transversalidade de Ciclos Ímpares de Fuleróides-(3, 4, 5, 6).* Rio de Janeiro: UFRJ/COPPE, 2017.

3. Acknowledgment

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