Drawing the Resonance Graphs of Catacondensed Benzenoid Graphs

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Introduction

Benzenoid graphs are defined as *2*-connected subgraphs of the hexagonal lattice. A benzenoid graph G is catacondensed if any triple of hexagons of *G* has empty intersection.

The concept of the resonance graphs models the interaction of two Kekulé structures (of catacondensed benzenoid hydrocarbons) that differ in the position of three double bonds.

The vertices of the resonance graph *R*(*G*) of the benzenoid hydrocarbon *G* are the Kekulé structures of *G*; two vertices of *R*(*G*) are adjacent if the corresponding Kekulé structures interact, that is if they differ in the position of just three double bonds.

Algorithm

We present the procedure Draw by means of which the resonance graph *R*(*G*) of the catacondensed benzenoid graph *G* is visualized.

Procedure **Draw**;
Input: *R*(*G*)
Output: visualization of *R*(*G*)

begin
1. Draw Line
2. **for** all vertices *v* of *R*(*G*) **do**
2.1 **for** all unvisited vertices *u* adjacent to *v* **do**
2.1.1 **if** number of visited vertices adjacent to *u* ≥ *2* **then**
2.1.2 Determine coordinate of *u* using paralelogram rule
2.1.3 **Else**
2.1.4 Determine coordinate of *u* with coordinates table
2.1.5 **If** coordinate does not satisfy constraints **then**
2.1.6 Visualization := unsuccessful
2.1.7 Exit;
2.2 **End For;**
3. **End For;**
4. Visualization:= successful
End.

The procedure Draw first calls an auxiliary procedure Draw Line. The procedure uses the benefits of the decomposition theorem as well as of the canonical binary coding introduced in [1]. The decomposition theorem shows that the resonance graph of a catacondensed benzenoid graph *G* (with respect to an edge *e* of *G*) is "almost" isomorphic to the Cartesian product of a certain smaller graph *Y* and a path on *n+1* vertices. More precisely, the resonance graph of a catacondensed benzenoid graph compose *n* copies of *Y* and a subgraph *X* of *Y*. The canonical coding assigns a binary string s to every *1*-factor of a catacondensed benzenoid graph. Every string s contains a prefix *11...100...0* of length *n*, where the number of *1*'s corresponds to the position of a copy of *Y* in *R*(*G*). In other words, the *1*-factors of the "first" copy of *Y* receive the prefix *00...0*, whilst the *1*-factors of *X* receive the prefix *11...1*.

R(*G*) is represented in R^3 with each copy of *Y* (as well as *X*) in a separate plane. Result of Draw Line is a straight line starting with vertex *00...0*, which determines the final 3D look of *R*(*G*) and the distance between planes.

In the main for loop of the procedure all vertices of *R*(*G*) are examined and searched for their adjacent unvisited vertices *u*. The vertex *u* is checked, whether it has at least two already visited vertices. If it does, then step 2.1.2. is executed and the coordinates of the vertex *u* are determined using paralelogram rule. Let *a* and *b* be already visited vertices adjacent to *u* and let *c* be the common neigbour of *a* and *b*. Coordinates of *u* are then determined as illustrated in Fig. 1.

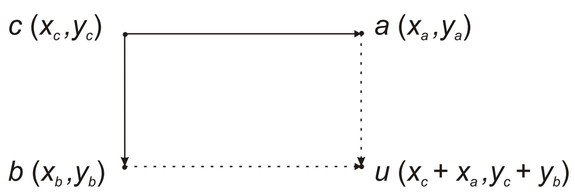


Figure 1: Paralelogram rule

If vertex *u* does not have at least two visited adjacent vertices, then new coordinate is determined with *coordinates table* (figure 2a), which contains posible coordinates of vertex *u* relative to vertex *v*. Coordinate of vertex *u* is determined in consecutive order, thus changing the order in *coordinates table* results in different representation of *R*(*G*).

In step 2.1.5 algorithm checks, whether computed coordinate satisfies constraints or not. It is checked, if computed vertex coordinate overlaps some other vertex or lies on some edge of *R*(*G*). If they do not, then the attempt to visualize *R*(*G*) fails.

Procedure is successful, when appropriate coordinate for all vertices of *R*(*G*) is found.

	x_u	y_u
u_1	x_v + |edge|	y_v
u_2	x_v	y_v + |edge|
u_3	x_v - |edge|	y_v
u_4	x_v	y_v - |edge|
u_5	x_v + |edge|/4	y_v + |edge|/4
⋮	⋮	⋮

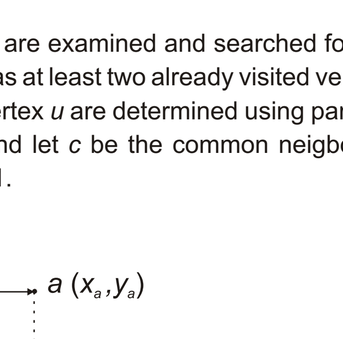
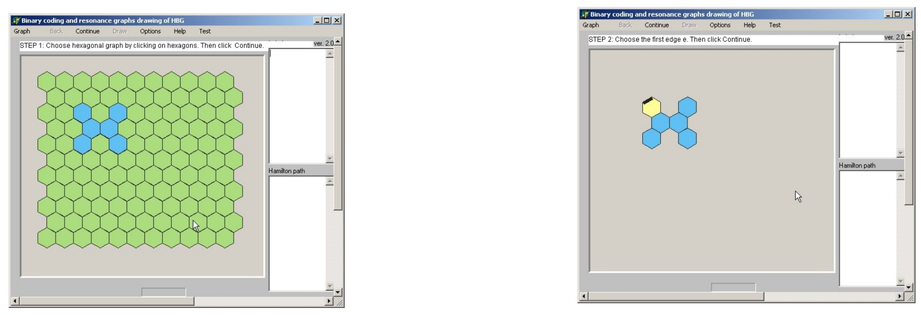


Figure 2: Coordinates table and its planar representation

Computer program

Program performs the visualization in three stages. First catacondensed benzenoid graph *G* is selected by clicking on green hexagons (Figure 3a). In the second phase an edge *e* of *G* that determines the decomposition of *R*(*G*) is chosen (Figure 3b). Finally, the computer program draws a resonance graph of selected catacondensed benzenoid graph (Figure 3c).



(a) (b)

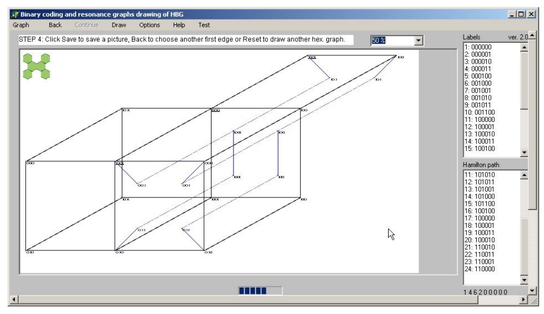
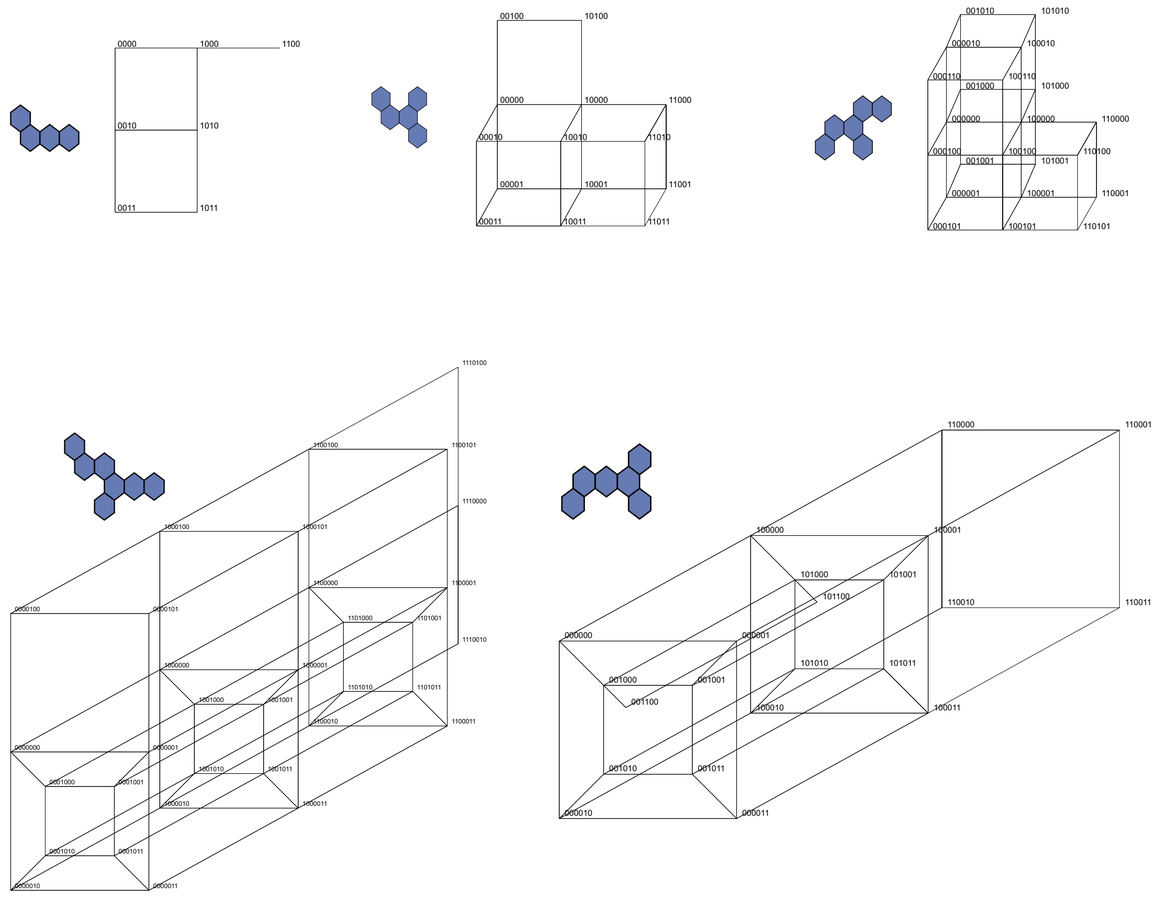


Figure 3: Program screenshots

Examples

Some examples are presented, each showing catacondesed benzenoid graph and its corresponding resonance graph.



5. References

[1] S. Klavžar, A. Vesel, P. Žigert, On resonance graphs of catacondensed hexagonal graphs: Structure, coding, and Hamilton path algorithm. Match (Krag.), 49 (2003).
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[5] D.L. Kreher, D. R. Stinson, Combinatorial algorithms: Generation, Enumeration and Search (CRC Press, Boca Raton, 1999).