communications in mathematical
match
and in computer chemistry

no. 48, February 2003
MATCDY (48) 163- 177 (2003)

ISSN 0340 - 6253

Backtrack search and look-ahead for the construction of planar cubic graphs with restricted face sizes

Gunnar Brinkmann
Fakultät für Mathematik
Universität Bielefeld
D 33501 Bielefeld, Germany
gunnar@mathematik.uni-bielefeld.de

Brendan D. McKay
Department of Computer Science
Australian National University
ACT0200, Australia
bdm@cs.anu.edu.au

Ulrike von Nathusius
Frankenallee 125–127
D 60326 Frankfurt/Main
ulrike.vn@web.de

Abstract

We describe two algorithms for the construction of simple planar cubic 3-connected graphs with all face sizes in some specified set; equivalently, simple triangulations of the plane with all vertex degrees in a specified set. Output of non-isomorphic graphs is achieved without explicit isomorphism testing. We also give some results obtained using the algorithms, including the numbers of fullerenes up to 200 vertices, and verification of a famous conjecture of Barnette up to 250 vertices.

Dedication

The first and third author want to express their gratitude for the honour of having met the great mathematician Horst Sachs and even more for the pleasure of having met the wonderful person Horst Sachs at several conferences.

Introduction

The degree $\deg(f)$ of a face f in a simple planar 3-connected cubic graph embedded in the plane is the number of edges in its boundary. It equals the degree of the corresponding vertex in the dual graph – in this case a simple triangulation of the sphere. We will use the word *map* to denote a graph embedded in the plane (equivalently the sphere; the infinite face is not regarded as special), and will always assume the absence of multiple edges and loops whether we use the adjective *simple* or not.

Many problems in mathematics and chemistry (see e.g. [2, 3, 7, 9, 11, 12]) deal with maps of constant vertex degree where certain face degrees are permitted or forbidden. That is, there is a set $S = \{f_1, \ldots, f_k\} \subseteq \mathbb{N}$ such that all face degrees are required to be in S. For example, the well-known fullerenes (see [10]) can be defined as cubic planar maps whose faces are all pentagons or hexagons ($S = \{5, 6\}$). We will restrict ourselves to what is probably the most important case here, namely cubic maps. Let us refer to planar cubic maps with all face sizes in S as *S-maps*, and their dual triangulations as *S-triangulations*. In order to check conjectures for given S up to maps of a certain size or determine the energetically best molecule corresponding to an S-map with a given number of vertices (atoms), it is useful to have complete lists of all non-isomorphic S-maps for the number of vertices in question available.

Unfortunately, the construction of S-maps is a very difficult task if S is very small. The best known solution so far is given in [5]. The algorithms described there use a database of patches containing only faces with sizes in S and try to assemble cubic or quartic maps from them. Unfortunately no necessary and sufficient criteria are known to determine which patches occur in maps of a given order and which do not. The algorithm described in [5] is focused on the most difficult case: that where few face sizes are allowed. The number of non-isomorphic structures generated per second is low compared to generators for easier classes. If many face sizes are allowed, the approach is inefficient and unfortunately it also requires a lot of memory for the database of patches.

The *plantri* program, see [6], can list planar triangulations or their duals, that is cubic 3-connected planar maps, very efficiently (several hundred thousand non-isomorphic structures per second). It also contains special construction routines for the important triangulation classes where 3-gons are forbidden, 3-gons and 4-gons are forbidden, or all odd-degree faces are forbidden.

In the case where S matches one of these built-in classes apart from a small number of additional forbidden face degrees, good performance can be obtained by simply filtering from the output those maps having a face of forbidden degree.

In this article we present a method based on *plantri*'s code for generating all triangulations which is often much better than output filtering when S is not of the form just described. This program is called *plantri_ad* and can be obtained together with *plantri*. It works by pruning the internal search process used by *plantri* to reduce the number of intermediate graphs that cannot lead to an output with the desired face sizes. In principle a similar method could be used together with the other construction methods employed by *plantri* (of which we mentioned some above) but that is a task for a later paper.

Plantri basics

Plantri [6] is a computer program to constructively enumerate planar triangulations and other classes of planar graphs. The present version of *plantri_ad* uses the *plantri* code for generating 3-connected planar triangulations. This uses a method going back to Eberhard, Steinitz and Rademacher in [8] and [14]. Starting from an embedding of K_4, the following three operations are recursively applied.

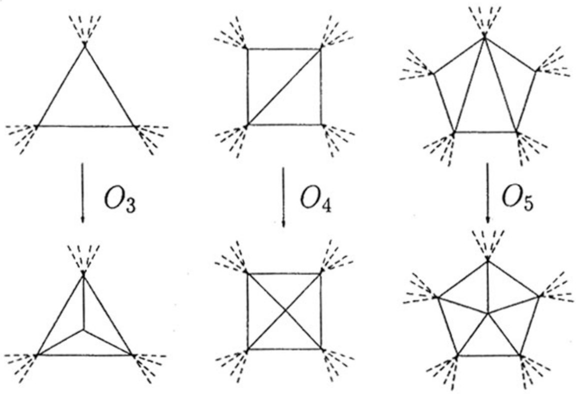

Figure 1:
The construction operations

At every step a new vertex of degree 3 is inserted into a face (operation O_3), a vertex of degree 4 is inserted into the quadrangle obtained by deleting an edge (O_4) or a vertex of degree 5 is inserted into the pentagon obtained by deleting two edges on the same face (O_5).

Of course most triangulations can be constructed (up to isomorphism) by many different sequences of these operations, so isomorph rejection methods have to be applied if we don't want isomorphic outputs. We use the *canonical construction path* method described in [13]. In this method there is a rooted *search tree* whose nodes are triangulations. Each node is either **accepted** or **rejected**. The root of the tree is the starting graph K_4, which is accepted. Recursively, rejected triangulations or triangulations of the desired output size have no children in the search tree. Accepted triangulations smaller than the output size have as children all the triangulations which can be formed by applying one of the operations O_3–O_5. These children may be either accepted or rejected. These definitions imply that the accepted triangulations form a connected subtree of the search tree; that is, all the ancestors of an accepted triangulation are also accepted.

The exact criteria for accepting or rejecting each triangulation are not important for our present purposes. However, we note two important implications of the criteria. First, there is exactly one accepted triangulation in each isomorphism class of simple planar triangulations of the output size. Second, a child formed by operation O_m is always rejected if it doesn't have minimum degree m (but the converse is not necessarily true).

Of course an efficient implementation will attempt to not construct children which will anyway be rejected. A brief summary of the approach taken by *plantri_ad* is that it also tries to not construct children which cannot have accepted descendants in the desired output class.

Applying degree restrictions

We are considering the generation of planar triangulations with n vertices, all vertex degrees being in S, for some $S \subseteq \mathbb{N}$ that will remain constant throughout this section. For $k \in \mathbb{N}$, a vertex of degree k will be called a k-vertex and the number of k-vertices in a graph G will be denoted by $n_k(G)$.

The following observations will be used repeatedly in this section. Note that the triangulation resulting from an operation O_m is regarded as having the same vertex set as its parent, except for one new vertex (chosen to be the obvious one).

Lemma 1 *Given a triangulation $G = (V, E)$, and an accepted child G' of G constructed by an operation O_m, $3 \le m \le 5$, the following hold.*

(1) *If $m \neq 5$, then $\forall v \in V$ we have $\deg_G(v) \le \deg_{G'}(v)$.*

(2) *If $m = 5$, then $\forall v \in V$ we have $\deg_G(v) - 1 \le \deg_{G'}(v)$, with equality holding for exactly one vertex $v \in V$.*

(3) *If $m \neq 4$ and $G \neq K_4$, then $n_3(G) \le n_3(G')$.*

(4) *If $m = 4$ and $G \neq K_4$, then $n_3(G) - 2 \le n_3(G')$, with equality holding only if $n_3(G) = 2$ and the two 3-vertices are in adjacent faces.*

Proof: Claims (1), (2) and (4) are obvious from the operations. Claim (3) is true in the case $m = 5$ because the fact that G' is accepted means its minimum degree is 5 and hence that the minimum degree of G is at least 4. Thus $n_3(G) = n_3(G') = 0$ in that case. For claim (3) in the case $m = 3$, note that a triangulation that is not K_4 cannot have two vertices of degree 3 on the same face; hence O_3, which adds a new vertex of degree 3, can increase the degree of at most one vertex from 3 to 4. ■

Definition 1 *If $G \neq K_4$ is a triangulation such that $n_3(G) \geq 3$, or $n_3(G) = 2$ and the two 3-vertices are not in adjacent faces, then G is called an* only-O_3-graph.

The following corollary gives us a first bounding criterion for the case that $3 \notin S$: an only-O_3-graph can be discarded without losing any S-triangulations because all of its accepted descendants have a vertex of degree 3.

Corollary 1 *If G is an only-O_3-graph, then only children made using O_3 can be accepted, and those accepted children are also only-O_3-graphs.*

Proof: Suppose that G' is the result of applying O_3 to G. By (3), $n_3(G') \geq 2$. If $n_3(G') = 2$ yet its two 3-vertices lie in adjacent faces, it is easy to see that $n_3(G) = 2$ and its two 3-vertices also lay in adjacent faces (contradicting the assumption that G is an only-O_3-graph). Hence, by induction, all the descendants of G formed using only O_3 are only-O_3-graphs.

A child of an only-O_3-graph formed using O_4 will be rejected by (4), while one formed using O_5 will be rejected because its minimum degree is less than 5. ■

The next lemma gives a second criterion that can detect some additional triangulations without accepted descendants that are S-triangulations in the case that $3, 4 \notin S$. Define $s_{3,4}(G) = 2n_3(G) + n_4(G)$. If a triangulation has n_0 vertices and we want to construct triangulations on n vertices without vertices of degree 3 or 4, then G can be discarded if $s_{3,4}(G) > n - n_0 + 1$.

Lemma 2 *Let G be a triangulation and let G' be an accepted child of G constructed using O_m. If $m \in \{3, 4\}$ or $s_{3,4}(G) > 2$, then $s_{3,4}(G') \geq s_{3,4}(G) - 1$.*

Proof: This is obvious from the operations. ■

In the following we will discuss bounding criteria that can be applied in a more general context. The first is a consequence of Lemma 2. Define $\Delta = \max S$ and $o(G) = \sum_{v \in V(G), \deg(v) > \Delta} (\deg(v) - \Delta)$. (If S is infinite, $\Delta = \infty$ and $o(G) = 0$.)

Lemma 3 *If $o(G) > 0$ then, for every S-triangulation G' that is an accepted descendant of G, we have $|V(G')| \geq |V(G)| + s_{3,4}(G) - 2 + o(G)$.*

Proof: Since $o(G') = 0$, and since only O_5 can decrease the value of $o(G)$ (and only by one, see Lemma 1(2)), we need at least $o(G)$ operations O_5. As long as $s_{3,4}(G) > 2$, no operation O_5 can give an accepted triangulation, so because of Lemma 2 at least $s_{3,4}(G) - 2$ operations O_3 or O_4 must be performed before the first operation O_5. Since with every operation we get one new vertex, an accepted S-triangulation that is a descendant of G must have at least $|V(G')| \geq |V(G)| + s_{3,4}(G) - 2 + o(G)$ vertices. ■

For only-O_3-graphs it is easy to see that unless $o(G) = 0$ we need not construct any descendants, or to be exact:

Lemma 4 *If for an only-O_3-graph G we have $o(G) > 0$, then no accepted descendant of G will be an S-triangulation.*

In fact this lemma is a special case of what follows.

Definition 2 *For $k \in \mathbb{N}, k \geq 3$, define*

$$\begin{aligned} e_\uparrow(k) &= \min(\{(k'-k) \mid k' \in S, k' \geq k\} \cup \{\infty\}), \text{ and} \\ e_\downarrow(k) &= \min(\{(k-k') \mid k' \in S, k' \geq 5, k' \leq k\} \cup \{\infty\}). \end{aligned}$$

For some arbitrary $x \in \mathbb{R}$, which we will choose later depending on the case, define

$$\text{deg\_err}_x(k) = \min(e_\uparrow(k), (1+x)e_\downarrow(k)).$$

For a triangulation G and $v \in V(G)$, define

$$\text{err}_x(G,v) = \begin{cases} e_\uparrow(\deg_G(v)), & \text{if } G \text{ is an only-}O_3\text{-graph} \\ \text{deg\_err}_x(\deg_G(v)), & \text{otherwise,} \end{cases}$$

and

$$\text{error}_x(G) = \sum_{v \in G} \text{err}_x(G,v).$$

Lemma 5 *The following inequalities hold:*

$$\begin{aligned} \text{deg\_err}_x(k+1) &\geq \text{deg\_err}_x(k) - 1 & \forall k \geq 3; \\ \text{deg\_err}_x(k-1) &\geq \text{deg\_err}_x(k) - (1+x) & \forall k \geq 6,\ x \geq 0. \end{aligned}$$

Proof: If $\text{deg\_err}_x(k+1) = 0$, then clearly $\text{deg\_err}_x(k) \leq e_\uparrow(k) = 1$, so $\text{deg\_err}_x(k+1) \geq \text{deg\_err}_x(k) - 1$ in that case. On the other hand, if $\text{deg\_err}_x(k+1) \neq 0$, then $e_\uparrow(k+1) \neq 0$, $e_\downarrow(k+1) \neq 0$. Furthermore, $\text{deg\_err}_x(k+1) = \min(e_\uparrow(k+1), (1+x)e_\downarrow(k+1)) \geq \min(e_\uparrow(k)-1, (1+x)e_\downarrow(k)+(1+x)) \geq \min(e_\uparrow(k), (1+x)e_\downarrow(k)) - 1 = \text{deg\_err}_x(k) - 1$.

If $\text{deg\_err}_x(k-1) = 0$, then clearly $\text{deg\_err}_x(k) \leq (1+x)e_\downarrow(k) = 1+x$ (since $k \geq 6$), so $\text{deg\_err}_x(k-1) \geq \text{deg\_err}_x(k) - (1+x)$ in that case. On the other hand, if $\text{deg\_err}_x(k-1) \neq 0$, then $e_\uparrow(k-1) \neq 0$, $e_\downarrow(k-1) \neq 0$. Furthermore, $\text{deg\_err}_x(k-1) = \min(e_\uparrow(k-1), (1+x)e_\downarrow(k-1)) \geq \min(e_\uparrow(k)+1, (1+x)e_\downarrow(k) - (1+x)) \geq \min(e_\uparrow(k), (1+x)e_\downarrow(k)) - (1+x) = \text{deg\_err}_x(k) - (1+x)$. ■

Lemma 6 *If G is a triangulation and G' is an accepted child of G, then the following hold.*

- *If G' was constructed from G by O_3, then* $\text{error}_x(G') \geq \text{error}_x(G) - 3 + \text{deg\_err}_x(3)$.
- *If G' was constructed from G by O_4, then* $\text{error}_x(G') \geq \text{error}_x(G) - 2 + \text{deg\_err}_x(4)$.
- *If G' was constructed from G by O_5, then* $\text{error}_x(G') \geq \text{error}_x(G) - (3+x) + \text{deg\_err}_x(5)$.

Proof: If G is an only-O_3-graph, the result follows directly from Corollary 1 and the definitions.

Now suppose G, G' are not only-O_3-graphs. In case G' was constructed by O_3, there are vertices v_1, v_2, v_3 whose degree in G' is greater by one than their degree in G. Let the newly added vertex be v.

Then we have $\text{error}_x(G') = \sum_{w \in G'} \text{err}_x(G', w) =$
$\sum_{w \in V(G)-\{v,v_1,v_2,v_3\}} \text{err}_x(G', w) + \text{err}_x(G', v) + \text{err}_x(G', v_1) + \text{err}_x(G', v_2) + \text{err}_x(G', v_3)$.
By Lemma 5 for $i \in \{1,2,3\}$ we have $\text{err}_x(G', v_i) = \text{deg\_err}_x(\deg_{G'}(v_i)) \geq$
$\text{deg\_err}_x(\deg_G(v_i)) - 1 = \text{err}_x(G, v_i) - 1$, so $\text{error}_x(G') \geq \text{error}_x(G) - 3 + \text{deg\_err}_x(3)$.

In the same way we get the results for O_4 and O_5. Note that for O_5 the only vertex w with $\deg_G(w) > \deg_{G'}(w)$ must have degree at least 6 in G, since otherwise G' would not have been accepted because the last vertex added does not have minimal degree.

If G' is an only-O_3-graph the result follows from the previous case, since $\text{error}_x(G')$ is at least as large as the value obtained when taking $\text{deg\_err}_x(\deg(v))$ instead of $e_\uparrow(\deg(v))$ for every vertex v.

■

Definition 3 *For $x \geq 0$, define* $m_x = \max\{3 - \text{deg\_err}_x(3), 2 - \text{deg\_err}_x(4), 3 + x - \text{deg\_err}_x(5)\}$.

Corollary 2 *If G is a triangulation with n' vertices and* $\text{error}_x(G) > m_x(n - n')$ *for any x, n, then no accepted descendant of G with n vertices is an S-triangulation. (So G can be discarded.)*

Proof: Since the error of an S-triangulation is clearly 0, this follows by induction from the previous lemma. ■

Given S, the only variable parameter in m_x is x. In order to get a powerful bounding criterion, we have to choose x in a way that the fraction $\text{error}_x(G)/m_x$ is as large as possible. While it is difficult to control the effect of x on $\text{error}_x(G)$, since it depends very much on the degrees of the vertices in G, it is easy to control the effect on m_x. So we choose x maximal in a way that m_x still is as small as possible, that is

$$x = \begin{cases} e_\uparrow(5) - 1 & \text{if } 3, 5 \notin S \\ e_\uparrow(5) & \text{otherwise,} \end{cases}$$

Since for all x we have $\text{deg\_err}_x(5) = e_\uparrow(5)$ this gives

$$m_x = \begin{cases} 2 & \text{if } 3, 5 \notin S \\ 3 & \text{otherwise.} \end{cases}$$

Other values of x might potentially be used instead (or as well) but we have found only one case where it improves the efficiency consistently. If S includes 5 but at most two values greater than 5, it helps a little to use $x = 1$ in addition to the value given above.

Lemma 7 *If G is an only-O_3-graph, $I \subseteq V(G)$ an independent set and* $\sum_{v \in I} e_\uparrow(\deg(v)) > n - |V(G)|$, *then no accepted descendant of G with n vertices is an S-triangulation.*

Since one application of O_3 can change the degree of only one element of the independent set, the result immediately follows. It would be much too expensive to compute the independent set with the largest sum of errors, so we just rank the vertices with respect to their errors (giving a higher rank to the ones with smaller degree if the error is the same) and construct an independent set by recursively including the highest ranked vertex that is no neighbour of a vertex already in the set.

The various conditions we have described have been implemented as bounding criteria and inserted into the program *plantri*. For various parameters the results have been compared to filtering the output of *plantri* and to the results of the computer program *CPF* described in [5] which can also construct complete lists of S-triangulations. They were in complete agreement. Some example results and running times are given in the appendix.

The special case $S = \{3, 4, 5, 6\}$

As can be seen from the tables at the end, and could be predicted from the previous section, the generation rate is not very high in those cases where S is small compared to the set of all theoretically possible vertex degrees.

Of course, it is to be expected that special purpose algorithms will do better in some specific cases. One such example is $S = \{3, 4, 5, 6\}$.

The theorem by Eberhard, Steinitz and Rademacher does not only say that every triangulation can be constructed from K_4 by O_3, O_4 and O_5, equivalently that every triangulation except K_4 can be reduced by the inverse operations O_3^{-1}, O_4^{-1} and O_5^{-1}. In fact, if the minimum degree of a triangulation G other than K_4 is m, then G can be reduced by O_m^{-1} centered at v for any vertex of degree m.

Since only O_5^{-1} can increase a vertex degree, we get the following lemma.

Lemma 8 *Every $\{3, 4, 5, 6\}$-triangulation can be constructed from a $\{5, 6\}$-triangulation or from K_4, using only the operations O_3 and O_4.*

The set of $\{5, 6\}$-triangulations is the set of duals of the famous fullerenes, see [10]. They represent a special class of spherical carbon atoms. For this class a special purpose generation algorithm has already been developed and implemented, see [4].

Using this generator *fullgen*, we implemented a special version of plantri – *plantri_md6* – that uses duals of fullerenes generated by *fullgen* as starting graphs and constructs the class of $\{3, 4, 5, 6\}$-triangulations out of them. Sample results are given in the tables at the end.

An application of *plantri_md6* was reported in [1]. A famous conjecture of Barnette is that all $\{3, 4, 5, 6\}$-maps are hamiltonian. We generated these cubic graphs using *plantri_md6* as far as 176 vertices and found them to be all hamiltonian. For this paper, we have extended the computation to 250 vertices with the same outcome. It is helpful to note that O_3 preserves hamiltonicity of the dual cubic graph, so testing only $\{4, 5, 6\}$-maps is sufficient. Lemma 1 can be used to restrict the generation to $\{4, 5, 6\}$-maps with reasonable efficiency.

number of vertices	number of faces	min. degree 3	min. degree 4	min. degree 5	total
4	4	1	0	0	1
5	6	1	0	0	1
6	8	1	1	0	2
7	10	4	1	0	5
8	12	8	2	0	10
9	14	11	4	0	15
10	16	23	7	0	30
11	18	34	10	0	44
12	20	54	22	1	77
13	22	83	32	0	115
14	24	125	58	1	184
15	26	174	92	1	267
16	28	267	151	2	420
17	30	365	227	3	595
18	32	509	368	6	883
19	34	706	530	6	1 242
20	36	963	805	15	1 783
21	38	1 270	1 158	17	2 445
22	40	1 708	1 695	40	3 443
23	42	2 204	2 373	45	4 622
24	44	2 876	3 354	89	6 319
25	46	3 695	4 595	116	8 406
26	48	4 708	6 340	199	11 247
27	50	5 925	8 480	271	14 676
28	52	7 491	11 417	437	19 345
29	54	9 255	15 049	580	24 884
30	56	11 463	19 832	924	32 219
31	58	14 083	25 719	1 205	41 007
32	60	17 223	33 258	1 812	52 293
33	62	20 857	42 482	2 385	65 724
34	64	25 304	54 184	3 465	82 953
35	66	30 273	68 271	4 478	103 022
36	68	36 347	85 664	6 332	128 343
37	70	43 225	106 817	8 149	158 191
38	72	51 229	132 535	11 190	19 4954
39	74	60 426	163 194	14 246	237 866

Table 1: $\{3,4,5,6\}$-triangulations listed with respect to their minimum degree.

number of vertices	number of faces	min. degree 3	min. degree 4	min. degree 5	total
40	76	71 326	200 251	19 151	290 728
41	78	83 182	244 387	24 109	351 678
42	80	97 426	296 648	31 924	425 998
43	82	113 239	358 860	39 718	511 817
44	84	131 425	431 578	51 592	614 595
45	86	151 826	517 533	63 761	733 120
46	88	175 302	617 832	81 738	874 872
47	90	200 829	735 257	99 918	1 036 004
48	92	231 042	870 060	126 409	1 227 511
49	94	263 553	1 029 114	153 493	1 446 160
50	96	300 602	1 209 783	191 839	1 702 224
51	98	341 960	1 420 472	231 017	1 993 449
52	100	388 673	1 659 473	285 914	2 334 060
53	102	438 795	1 937 509	341 658	2 717 962
54	104	496 961	2 249 285	419 013	3 165 259
55	106	559 348	2 612 410	497 529	3 669 287
56	108	629 807	3 015 386	604 217	4 249 410
57	110	706 930	3 483 289	713 319	4 903 538
58	112	792 703	4 002 504	860 161	5 655 368
59	114	885 137	4 600 343	1 008 444	6 493 924
60	116	990 929	5 257 856	1 207 119	7 455 904
61	118	1 102 609	6 019 580	1 408 553	8 530 742
62	120	1 227 043	6 849 385	1 674 171	9 750 599
63	122	1 363 825	7 805 813	1 942 929	11 112 567
64	124	1 513 612	8 846 570	2 295 721	12 655 903
65	126	1 673 568	10 041 875	2 650 866	14 366 309
66	128	1 853 928	11 335 288	3 114 236	16 303 452
67	130	2 045 154	12 821 597	3 580 637	18 447 388
68	132	2 255 972	14 415 241	4 182 071	20 853 284
69	134	2 485 363	16 248 586	4 787 715	23 521 664
70	136	2 732 106	18 211 371	5 566 948	26 510 425
71	138	2 998 850	20 454 113	6 344 698	29 797 661
72	140	3 295 090	22 845 386	7 341 204	33 481 680
73	142	3 606 102	25 587 469	8 339 033	37 532 604
74	144	3 944 923	28 486 985	9 604 410	42 036 318
75	146	4 316 997	31 808 776	1 0867 629	46 993 402

Table 2: $\{3,4,5,6\}$-triangulations listed with respect to their minimum degree.

number of vertices	number of faces	min. degree 3	min. degree 4	min. degree 5	total
76	148	4 711 036	35 313 024	12 469 092	52 493 152
77	150	5 135 792	39 315 257	14 059 173	58 510 222
78	152	5 599 064	43 529 293	16 066 024	65 194 381
79	154	6 091 434	48 339 503	18 060 973	72 491 910
80	156	6 621 013	53 361 973	20 558 765	80 541 751
81	158	7 198 926	59 117 687	23 037 593	89 354 206
82	160	7 800 960	65 110 206	26 142 839	99 054 005
83	162	8 460 776	71 938 170	29 202 540	109 601 486
84	164	9 168 331	79 041 731	33 022 572	121 232 634
85	166	9 917 770	87 147 815	36 798 430	133 864 015
86	168	10 711 602	95 517 629	41 478 338	147 707 569
87	170	11 590 678	105 090 744	46 088 148	162 769 570
88	172	12 491 728	114 936 802	51 809 018	179 237 548
89	174	13 478 996	126 169 796	57 417 255	197 066 047
90	176	14 518 876	137 732 540	64 353 257	216 604 673
91	178	15 638 778	150 895 746	71 163 435	237 697 959
92	180	16 807 692	164 343 816	79 538 725	260 690 233
93	182	18 100 327	179 751 990	87 738 289	285 590 606
94	184	19 400 142	195 420 726	97 841 157	312 662 025
95	186	20 854 463	213 287 224	107 679 684	341 821 371
96	188	22 358 888	231 489 556	119 761 030	373 609 474
97	190	23 978 453	252 233 786	131 561 725	407 773 964
98	192	25 642 259	273 226 012	145 976 654	444 844 925
99	194	27 515 451	297 264 739	159 999 441	484 779 631
100	196	29 367 163	321 450 518	177 175 662	527 993 343
101	198	31 444 918	349 098 646	193 814 634	574 358 198
102	200	33 551 307	376 999 846	214 127 713	624 678 866

Table 3: $\{3,4,5,6\}$-triangulations listed with respect to their minimum degree.

number of vertices	S	number of structures	time CPF	time plantri_ad	time plantri for all triangulations + filter	time plantri for restricted triangulations + filter
16	$\{3,6\}$	2	<0.01	0.02	58.7	
20	$\{3,6\}$	3	<0.01	0.53		
24	$\{3,6\}$	2	<0.01	37.0		
26	$\{3,6\}$	7	<0.01	317.2		
16	$\{5,7\}$	1	<0.01	0.07	58.7	(m5) <0.01
20	$\{5,7\}$	2	<0.01	8.59		(m5) <0.01
24	$\{5,7\}$	13	0.5	1 859.2		(m5) 0.2
16	$\{4,9\}$	2	0.1	<0.01	58.7	(m4) 0.3
21	$\{4,9\}$	5	25.1	0.26		(m4) 1391
26	$\{4,9\}$	24	9 266.8	46.0		
16	$\{3,4,9\}$	2	18.7	0.03	58.5	
20	$\{3,4,9\}$	67	7 439.3	2.1		
16	$\{4,5,7\}$	124	0.8	0.36	58.7	(m4) 0.35
20	$\{4,5,7\}$	3 188	66.5	55.2		(m4) 246
16	$\{4,6,10\}$	20	1.4	0.15	58.7	(b) 0.01
18	$\{4,6,10\}$	81	18.1	2.10		(b) 0.03
20	$\{4,6,10\}$	418	273.6	33.5		(b) 0.2
14	$\{3,4,6,8\}$	350	11.6	0.1	1.24	
16	$\{3,4,6,8\}$	2 948	239.2	1.87	58.7	
18	$\{3,4,6,8\}$	28 619		35.83	3 372.0	
20	$\{3,4,6,8\}$	299 290		714.5		
14	$\{4,5,6,8,9\}$	566	5.3	0.13	1.25	(m4) 0.02
16	$\{4,5,6,8,9\}$	8 313	140	2.8	62	(m4) 0.32
18	$\{4,5,6,8,9\}$	141 567		72		(m4) 8.21
12	$\{3,4,5,6,8,9\}$	1 597	15.1	0.03	0.03	
14	$\{3,4,5,6,8,9\}$	36 469	659.6	0.5	1.2	
16	$\{3,4,5,6,8,9\}$	913 789		15.8	59	
11	$\{3,4,5,6,7,8,10\}$	964	6.2	0.01	0.01	
12	$\{3,4,5,6,7,8,10\}$	5 000	47.5	0.05	0.04	
13	$\{3,4,5,6,7,8,10\}$	27 222	339.5	0.16	0.2	
15	$\{3,4,5,6,7,8,10\}$	883 460		5.5	8.2	
17	$\{3,4,5,6,7,8,10\}$	30 565 942		224.5	444.7	

Table 4: Numbers of simple triangulations and comparison of running times for various sets of allowed degrees. The running times are in seconds on a 700MHz Pentium III. In the last column (mx) stands for *restricted to triangulations with minimum degree x* and (b) stands for *restricted to triangulations with all vertices even degree.*

In Tables 1–3 we give the numbers of $\{3,4,5,6\}$-maps, $\{4,5,6\}$-maps, and $\{5,6\}$-maps (fullerenes) up to 200 vertices.

References

[1] R.E.L. Aldred, S. Bau, D.A. Holton and B.D. McKay. Nonhamiltonian 3-connected cubic planar graphs. *SIAM J. Discrete Math.*, 13:25–32, 2000.

[2] D. Babic and N. Trinajstic. Resonance energies of fullerenes with 4-membered rings. *Int. J. Quantum Chem.*, 55:309–314, 1995.

[3] G. Brinkmann and M. Deza. Lists of face-regular polyhedra. *Journal of Chemical Information and Computer Sciences*, 40:530–541, 2000.

[4] G. Brinkmann and A.W.M. Dress. A constructive enumeration of fullerenes. *Journal of Algorithms*, 23:345–358, 1997.

[5] G. Brinkmann, O. Heidemeier, and T. Harmuth. The construction of cubic and quartic planar maps with prescribed face degrees. to appear in Discrete Applied Mathematics.

[6] G. Brinkmann and B.D. McKay. Fast generation of non-isomorphic planar cubic graphs. in preparation, see `http://cs.anu.edu.au/~bdm/index.html`.

[7] O. Delgado Friedrichs, A.W.M. Dress, A. Müller, and M.T. Pope. Polyoxometalates: A class of compounds with remarkable topology. *Molecular Engineering*, 3:9–28, 1993.

[8] V. Eberhard. *Zur Morphologie der Polyeder*. Teubner, 1891.

[9] B. Grünbaum. *Convex Polytopes*. John Wiley & Sons, Ltd., London, New York, Sydney, 1967.

[10] H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl, and R.E. Smalley. C_{60}: Buckminsterfullerene. *Nature*, 318:162–163, 1985.

[11] J. Malkevitch. Polytopal graphs. In L.W. Beineke and R.J. Wilson, editors, *Selected Topics in Graph Theory*, volume 3, pages 169–188. 1988.

[12] D.E. Manolopoulos, J.C. May, and S.E. Down. Theoretical studies of the fullerenes: C_{34} to C_{70}. *Chemical Physics letters*, 181(2,3):105–111, 1991.

[13] B.D. McKay. Isomorph-free exhaustive generation. *Journal of Algorithms*, 26:306–324, 1998.

[14] E. Steinitz and H. Rademacher. *Vorlesungen über die Theorie der Polyeder*. Springer, Berlin, 1934.