Fast Generation of Fullerenes

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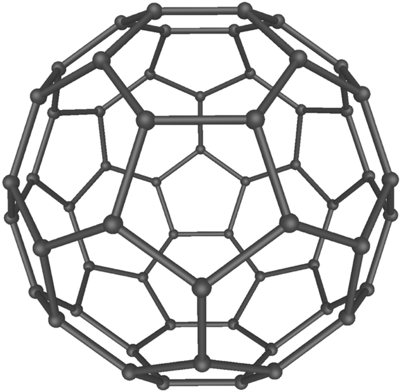
C_{60} buckyball



Discovered by Kroto et al. in 1985.

Fullerenes (combinatorially)

A *fullerene* is a cubic plane graph with faces of size 5 and 6.

Euler's formula implies that there are exactly 12 pentagonal faces.

History of generation of fullerenes

1991: Manolopoulos et al.

1991: Liu et al.

1993: Sah.

1995: Yoshida and Osawa.

But all incomplete or inefficient...

1997: Brinkmann and Dress.

- Complete.
- Efficient (program: *fullgen*).

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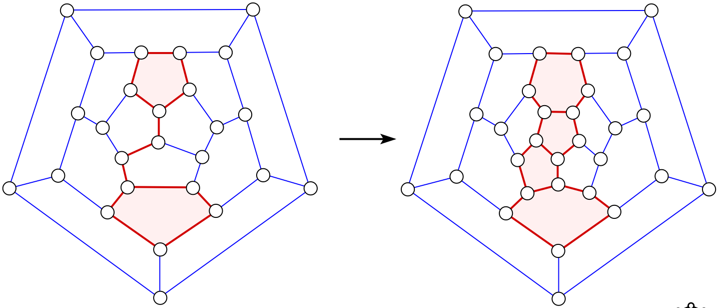
Construction of fullerenes

Growing fullerenes from smaller ones...

Example:



History of construction methods for fullerenes

2006: Brinkmann, Franceus, Fowler and Graver – up to 200 vertices, but fails in general.

2008: Hasheminezhad, Fleischner and McKay: described recursive structure for the class of all fullerenes.

Goal: turn the latter construction method into an efficient generation algorithm for fullerenes.

Why is this useful?

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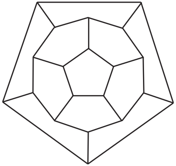
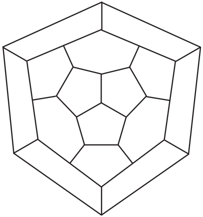
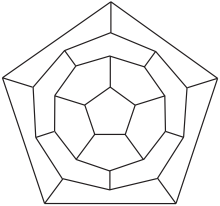
Starting points:



C_{20}



$C_{28}(T_d)$



$C_{30}(D_{5h})$

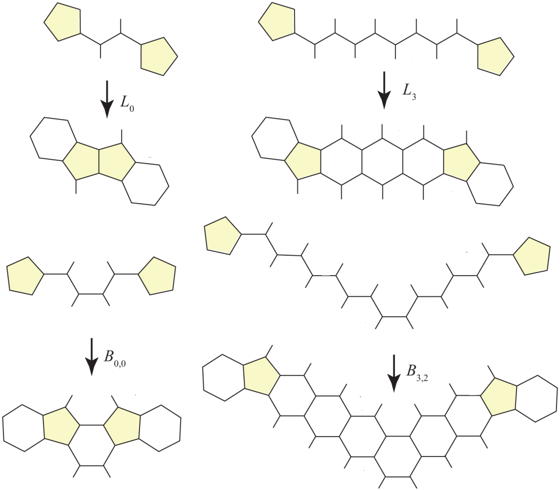
Construction operations

Extensions:

Note: no finite set of extensions is sufficient...
(proven by Brinkmann et al.)

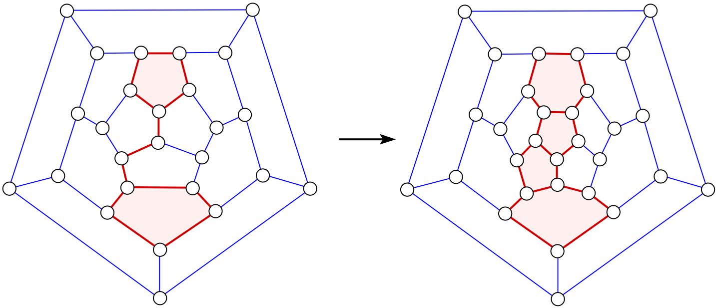
Construction operations

Extensions:



Construction operations

An L_0 extension:



Isomorphism rejection:

- Canonical construction path method.
- VERY roughly:
    - Don't perform extensions which are equivalent under the automorphism group of the fullerene.
    - Define a unique inverse operation (*canonical* reduction) which must be the last step in the construction and accept a fullerene only if it was constructed in this way.

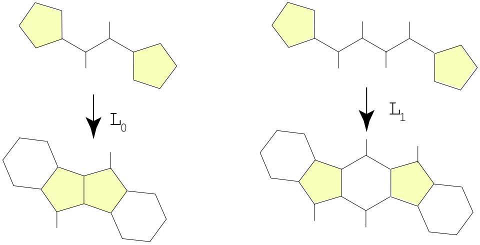
Optimizations

Problem: especially long extensions are expensive.

Goal: avoid performing (and searching for) long extensions.

Optimizations

- Give priority to short extensions.
  ⇒ *canonical* reduction is the shortest reduction...
  - Shortest reduction of fullerenes with 300 vertices:
    - L_0: 80.5%
    - L_1: 16.4%
    - other: 3.1%



Results that limit the length of the extensions:

Lemma (1)

If there is an L_0 reduction in G, all extensions (in one step) of G have an L_1, $B_{0,0}$ or shorter reduction.

Lemma (2)

If there are at least two L_1 reductions in G, all extensions (in one step) of G have an L_2, $B_{1,0}$ or shorter reduction.

$\Rightarrow$ So in these cases no need to perform long extensions since they won't be accepted...

Program based on this algorithm:

- Called *buckygen*.
- More than 3.5 times faster than *fullgen*.
- If generating all fullerenes in a range, speedup is much bigger.
  - E.g. 15 times faster than *fullgen* for generating all fullerenes with $n \in [290, 300]$ vertices.
- Contradicting results with *fullgen* lead to the detection of a (now fixed) bug in *fullgen*.
  - Missed fullerenes starting from 136 vertices.

caagt

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IPR fullerenes

IPR (Isolated Pentagon Rule) fullerenes are most interesting

as they are the chemically most stable ones.

n	fullerenes	IPR fullerenes	% IPR
20	1	0	–
...			
60	1 812	1	0.06
...			
100	285 914	450	0.16
...			
200	214 127 742	15 655 672	7.3
...			
250	1 712 934 069	230 272 559	13.4
...			
296	8 241 719 706	1 568 768 524	19.0
298	8 738 236 515	1 690 214 836	19.3
300	9 332 065 811	1 821 766 896	19.5

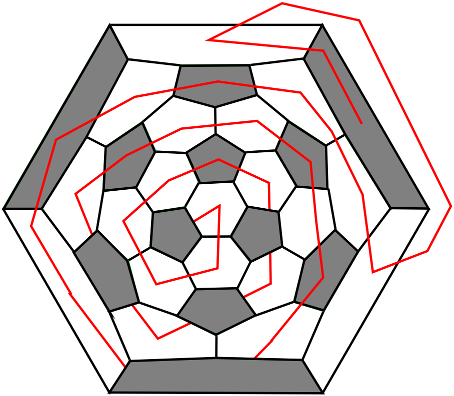
Growth rate $\sim n^9$ [Thurston]

More results

- Used *buckygen* to generate all non-isomorphic fullerenes up to 400 vertices.
- Independently confirmed by *fullgen* (new version) up to 380 vertices.

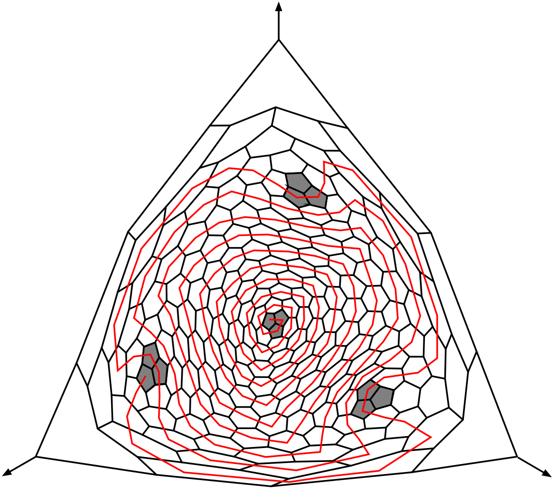
This allowed us to determine the smallest fullerene that does not have a *face spiral*...

What is a face spiral?



Face spirals

A face spiral which does not work:



Face spirals

- The spiral algorithm (1991 – Manolopoulos and Fowler).
  - Generates spiral codes.
  - Manolopoulos and Fowler gave an example of a fullerene with 380 vertices that does not allow any face spirals.
    - So the algorithm is incomplete.
- Later the IUPAC recommended face spirals as basis for fullerene nomenclature

So it would be interesting to know the smallest fullerene which does not have a face spiral...

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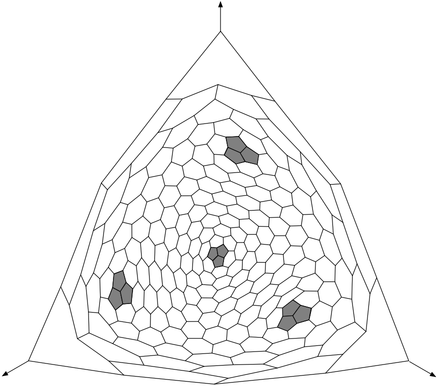
Face spirals

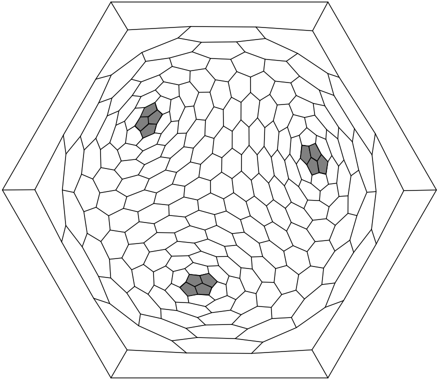
The smallest fullerene without a face spiral:



- Has 380 vertices.
- Is the counterexample from Manolopoulos and Fowler.

Face spirals

The second smallest fullerene without a face spiral:



- Has 384 vertices.
- Was also already known (constructed by Yoshida and Fowler – 1997).

More results

These 2 are the only fullerenes without a face spiral up to 400 vertices.

Conjecture (Barnette, 1969)

Every 3-connected cubic planar graph with maximum face size 6 is hamiltonian.

- We verified this up to 316 vertices.
- We verified this for fullerenes up to 336 vertices.

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- We verified this for fullerenes up to 336 vertices.

- Fullerenes can be downloaded from:
  - `http://hog.grinvin.org/Fullerenes`
- *Buckygen* is part of the *CaGe* software package:
  - `http://caagt.ugent.be/CaGe/`

Thanks for your attention!