CaGe

A virtual environment for studying some special classes of plane graphs

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Outline

What is CaGe?

a graphical user interface for a set of commandline generators and embedders

GUI

written in Java

generators and embedders

written in C and Java (any language will do)

User interface

Having a user interface
$\neq$
Being a user friendly program

Example

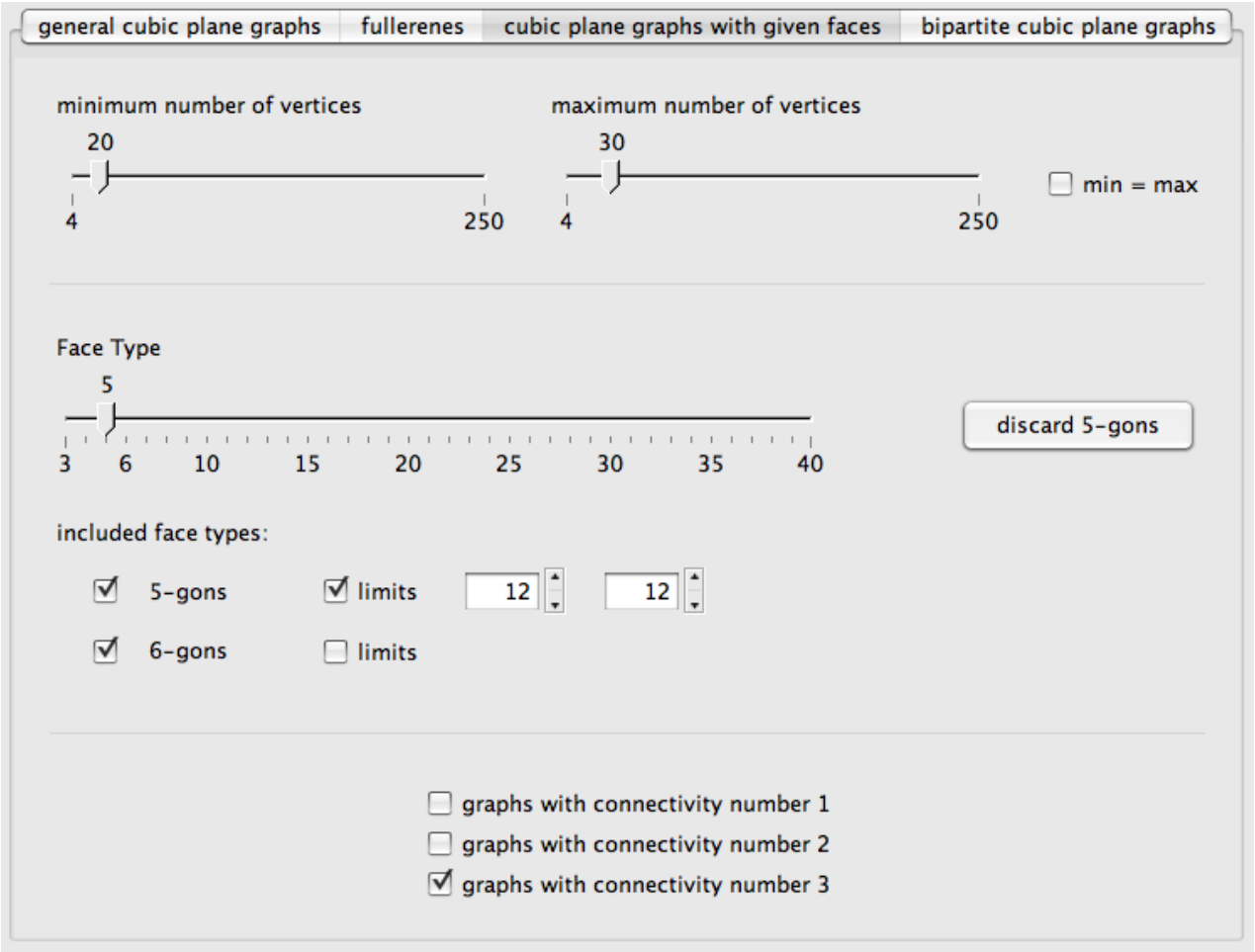
CGF

CGF is a generator for cubic plane graphs with given faces.

```
cgf -g 0 -output stdout -logfile stderr -save
0 -no_recover -topdown -outputmem 0 0 -v 30
-vs 20 -f 5 l12-12u -f 6 -mapcon 3
```

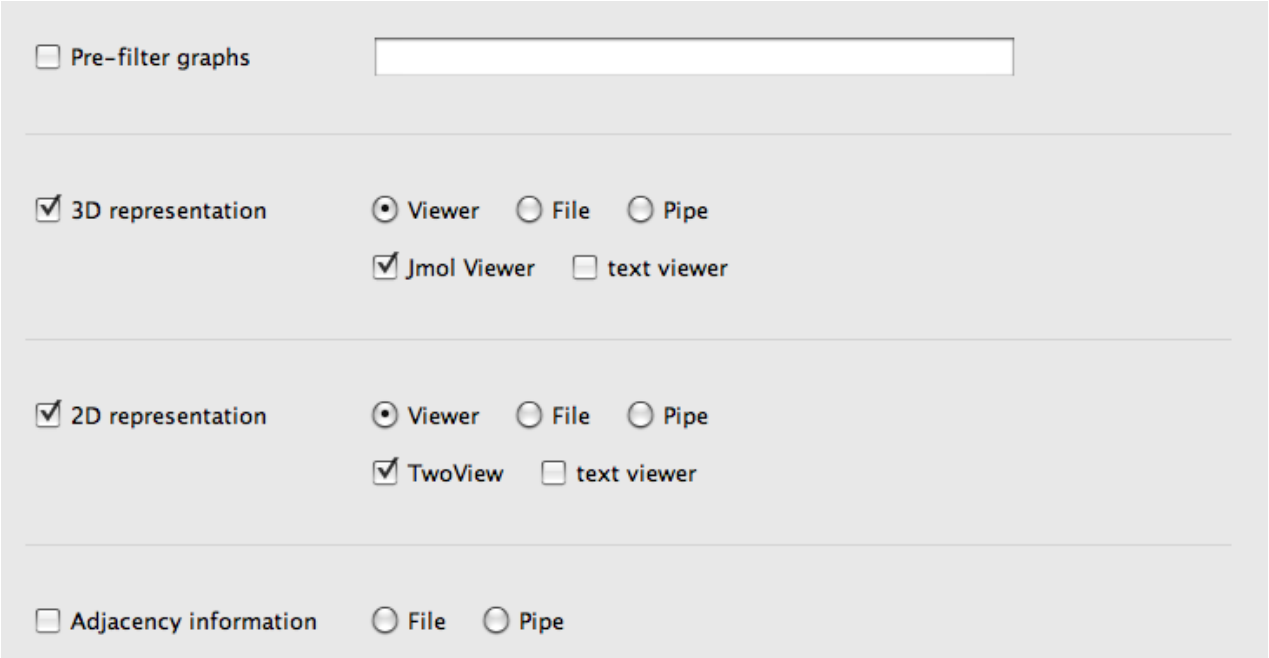
generates all 3-connected cubic plane graphs with 20 to 30 vertices, 12 pentagons and any number of hexagons.

And now with CaGe



Output

CGF and other generators in CaGe output a binary format, e.g. planar code.



Timeline

Some large steps...

Mid 90's	First version
2001	Java 1.1 version
March 2007	Mac OS X supported
June 2009	Java 5 version

... and a lot of small steps

- new generators and new embedders added
- user interface improved
- documented and cleaned up the code
- bugs fixes

Features

- visualization of the options
- checking of constraints on the parameters
- automatic selection of best suited generator
- easy browsing through the results of a generator
- embedding in 2D and 3D
- ...

Generators

3-regular plane graphs

- Fullerenes
- 3-regular plane graphs with given face sizes
- Bipartite 3-regular plane graphs
- General 3-regular plane graphs

4-regular plane graphs

- 4-regular plane graphs with given face sizes
- General 4-regular plane graphs

General plane graphs

Generators

Triangulations

- Triangulations with given vertex degrees
- Eulerian triangulations
- General triangulations
- Triangulations of the disk

Quadrangulations

- Quadrangulations with given vertex degrees
- General quadrangulations

Generators

Planar Polycyclic Hydrocarbons

- by formula (e.g. $C_{31}H_{17}$)
- by boundary formula (e.g. 222322223)
- by number of hexagons

Tubes and cones

- nanotubes
- nanocones

Embedders

- *embed*
  A general purpose embedder for fast embedding of planar graphs in the plane, on spheres and on tubes
- *NanotubeEmbedder*
  Specialized for nanotubes: aware of the cap of the nanotube
- *NanoconeEmbedder*
  Specialized for nanocones: aware of the number of pentagons and thus also of the aperture angle

Output

Three types of output after embedding

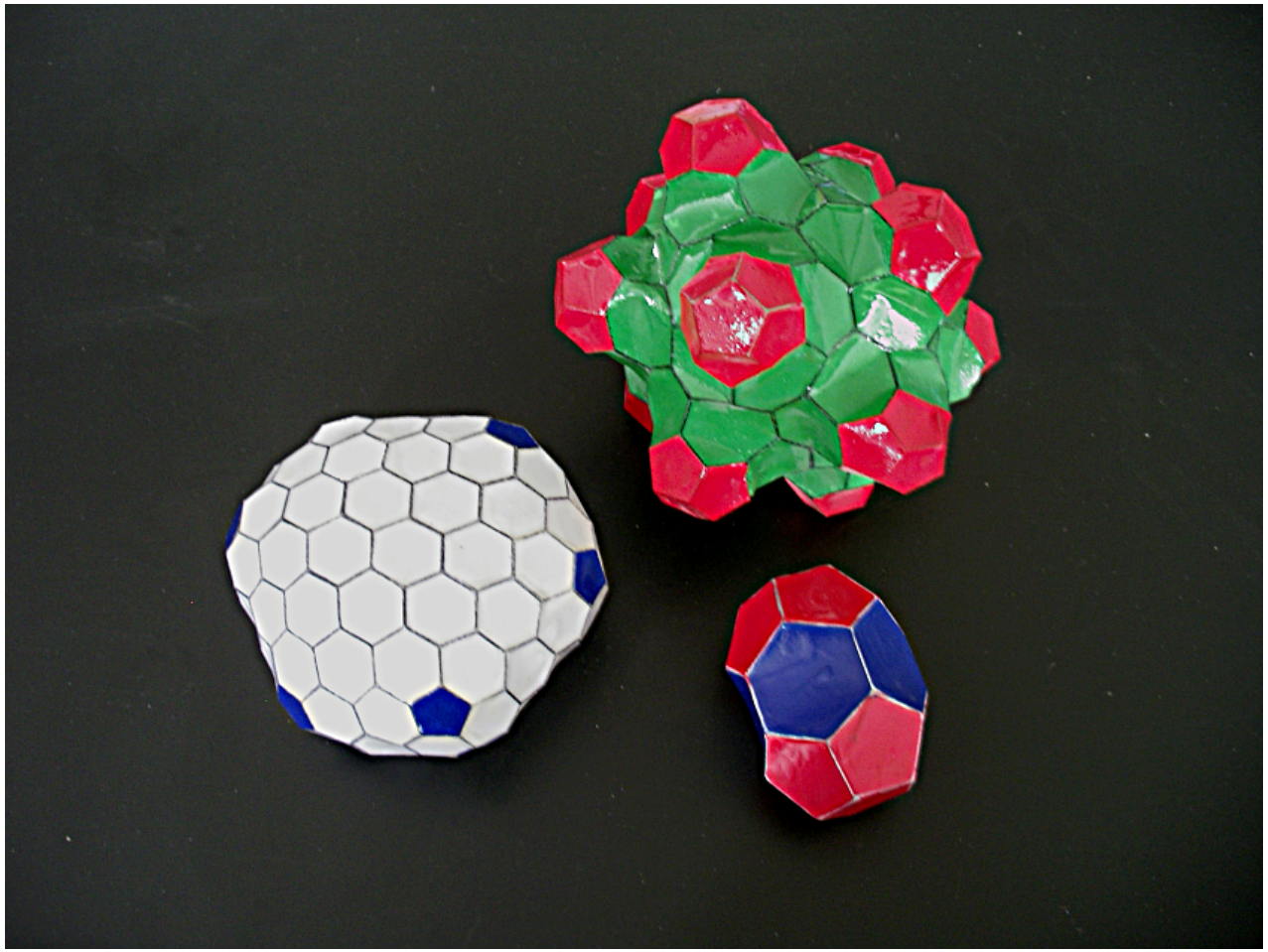
- adjacency information
  - text
- 3D representation
  - Jmol
  - Rasmol (when available)
  - text
- 2D representation (Schlegel diagram)
  - TwoView
  - text

Output

Other output options

- send graphs through filter first
- send output to a file
- send output to a pipe
- create unfolding of 3D representation

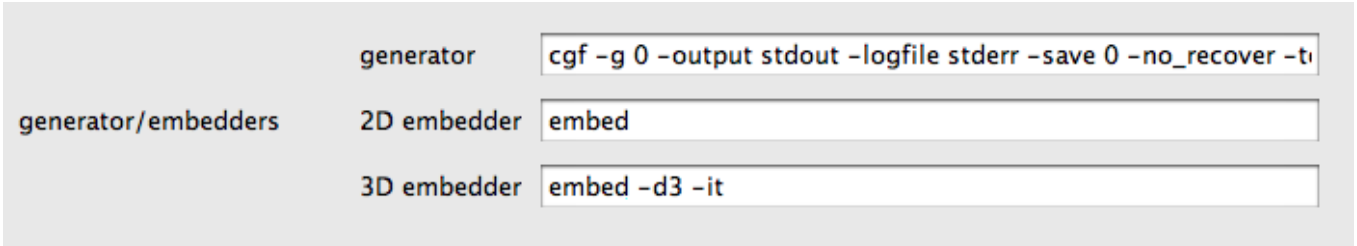
Unfolding of 3D representation



Command-line magic

Expert mode

Still possible to use unsupported generator/embedder features (or even custom embedders)



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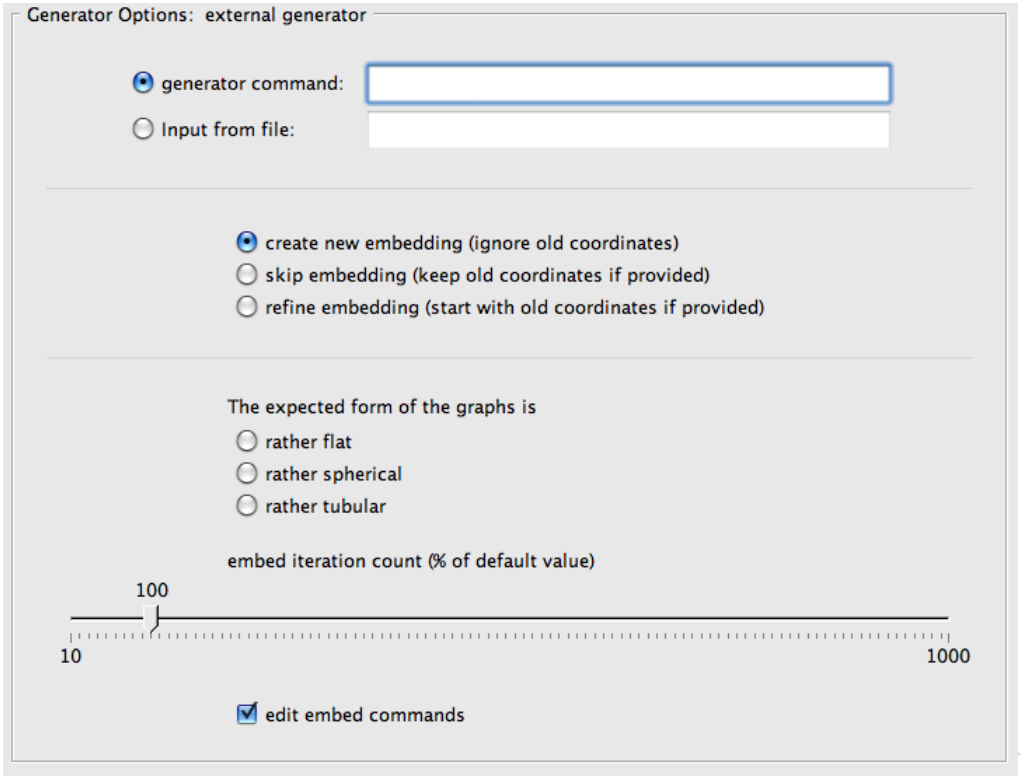
Command-line magic

External generator

Read graphs from a file or from a custom generator but still use wizard-like configuration for embedding



DEMO

Future work

- Improve embedders for non-fullerene-like structures
- Add more classes of graphs
- ... (suggestions?)

What can you do for CaGe?

- Use it!
- More important: Give feedback
- Programmers: contact us about adding programs to CaGe

People that contributed to CaGe

Simon Buelens
Gunnar Brinkmann
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Andreas Dress
Thomas Harmuth
Sebastian Lisken
Alexander Lust
Brendan McKay
Adriaan Peeters
Nico Van Cleemput
Ulrike von Nathusius

Thanks for your attention

Visit our websites:

http://caagt.ugent.be/CaGe

http://www.math.uni-bielefeld.de/∼CaGe