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CaGe – a Virtual Environment for Studying Some Special Classes of Plane Graphs

Nico VAN CLEEMPUT[1], Gunnar BRINKMANN[1],

Olaf DELGADO-FRIEDRICHS[2], Sebastian LISKEN[3], Adriaan PEETERS[1]

[1] *Applied Mathematics and Computer Science, Ghent University, Krijgslaan 281 – S9, B-9000 Ghent, Belgium*
[2] *The Supercomputer Facility, Australian National University Canberra ACT 0200, Australia*
[3] *Teichstr. 32, D-33615 Bielefeld, Germany*

CaGe (Chemical and Abstract Graph Environment) is an environment for generating and visualizing certain specialized classes of plane graphs with the emphasis on classes that are relevant in chemistry.

A first version of CaGe was described in [1] and since then CaGe was used by various researchers for much varying purposes (see [2],[3],[4] for example applications). The first version of CaGe was based on Tcl/Tk, but due to several problems with the speed and the development of Tcl/Tk, we decided that instead of repeatedly updating CaGe, we should better develop and support a new version based on Java. This Java based version was first released in 2001 and since then continuously updated (see [5] for the Changes History).

Compared to the version described in [1] the new version offers various new features and generators for more classes of graphs. Furthermore it is more portable now and runs under Unix/GNU-Linux and Mac OS X. Currently the development of CaGe is based in both Bielefeld and Ghent. Last year a major reworking of the code and the interface of CaGe was done: we made the interface which had grown organically during the years more uniform. At the same time we documented the code to allow for easier maintenance and extension.

A session with CaGe basically works as follows. You start by making a first coarse selection, followed by a refinement step. Next you set the parameters for the generator. Once these parameters have been set, CaGe will determine which generator to use. Mostly there is just one choice but for some cases (e.g. cubic graphs with given faces) there are multiple possibilities and the generator that is expected to be the most efficient one is chosen. The final step before the generator is started is to specify the output. CaGe has the option to first pipe the results of the generator through a filter program which may add extra restrictions on the graphs that weren't implemented in the original generator. The graphs can be drawn in 2 and 3 dimensions, an adjacency matrix can be given and even an unfolding of the 3 dimensional structure can be outputted. Any combination of these options is also possible. Currently CaGe has 3 embedders: one general embedder which uses different techniques and is described in [6], and two specialized embedders for nanocones and nanotubes. Once the generator is running you can browse through the results using the navigation window.

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