**AutoGraphiX, a software for computer aided graph theory**

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This talk will be dedicated to the presentation of the *AutoGraphiX* (*AGX*) software. First, an introduction on computer aided graph theory and the main softwares from that field will be given, followed by a description of the software and the main principles on which it is based. Its use will finally be illustrated by the mean of some application examples.

Computer aided graph theory started in the 1980's when *Graph* (D. Cvetkovic), *Graffiti* (S. Fajtlowicz), *Ingrid* (R.C. Brigham and R.D. Dutton) and *Graph Theorist* (S.L. Epstein) were developped.

*AGX* was developped in 1997, during G. Caporossi's PhD thesis under the guidance of P. Hansen. At that time, the first developpements of the Variable Neighborhood Search (VNS) were also occuring at GERAD by N. Mladenovic and P. Hansen. This synergy had a positive impact on *AGX*. Other computer aided graph theory software were developped later, like *Graphedron, GrinvIn* or *NewGraph* for example, but *AGX* is still the only one that uses optimization.

*AGX* is based upon the concept of graph invariant, a property which is preserved under all possible graph isomorphisms. The main characteristic of *AGX*, when comparing to other softwares, is the use of optimization to search for (supposed) extremal graphs (by minimizing or maximizing the value of a given invariant, eventually subject to some constraints). If parameters are used, this search leads to the identification of families of extremal graphs. Data mining techniques could then be applied to find some properties shared by those graphs and to propose conjectures. A graphical interface finally allows the researcher to test some ideas or to use the software as a tool to stimulate his intuition. The capability of AGX to compute easily and quickly the values of some invariants is very useful.

After the proof of concept with the original version, a second version of the software was developped between 2001 and 2007 (a *Windows* version was made available for public use in 2005 through the GERAD's website)*.* A new version of the software is currently being developped. It handles the optimization of values computed for each vertex and supports multi-objective optimization (collaboration with S. Majstorovic).

*AGX* has contributed to various fields in science, such as :

- Artificial intelligence : In his report as external examinator for G. Caporossi's thesis, H. Simon, Nobel price of Economics in 1978 and pioneer in the development of artificial intelligence software, described AutoGraphiX as an innovative software in artificial intelligence.

**-** Graph theory : It is not surprising to notice that one of the main applications of AGX is graph theory. It is now widely used across the world and the original paper describing AGX in 2000 was cited 94 times\*.

- Mathematical chemistry : AGX produced important results in the field of mathematical chemistry, among them, the study of molecular energy (which may be computed as a graph invariant). The paper in 1999 on that topic was cited 74 times\* and it clearly renewed the interest of the research community on that topic.

- Telecommunications : AGX was used to build graphs with some given desirable properties for a robust telecommunication network. Some further developpements are on the way.

\* *according to ISI web of science*