An up-to-date overview of free software and its makers

PROJECTS ON THE MOVE

Graphics can facilitate research into chemical compounds. The chemistry software, Avogadro, has no trouble handling the third dimension and has an intuitive interface that offers more than its share of functionality.

BY CARSTEN SCHNOBER

Chemistry is a science that imposes particularly exacting requirements on IT: Before researchers can start investigating complex molecular structures, they first need sophisticated software to visualize them. Without a three-dimensional view, it is easy to lose track of changes made to molecules. The free Avogadro [1] program (Figure 1) meets the challenge effectively and without any compromises to available features.

Famous Namesake

The chemistry program's name is a tribute to the Italian physicist and chemist Amedeo Avogadro, who created Avogadro's law in the 19th century; it states that equal volumes of perfect gases, at the same temperature and pressure, contain the same number of molecules. Avogadro also invented the constant that bears his name and that defines the number of elementary entities (usually atoms or molecules) in a physical quantity.

The developers, led by the project's initiator, Marcus D. Hanwell [2], are thus walking in the footsteps of a famous historical character. However, the main developer does have a PhD in physics from the University of Sheffield. He is also a KDE developer; no points for guessing that the Avogadro interface is based on Qt. Just like the underlying programming language, Python, the program not only runs on Linux, but also on Windows and Mac OS X. Version 0.9 now sees the project entering the beta phase.

Molecular Editor

Avogadro is easy to use. One of the stated aims of the project is to make it possible for students, and not just advanced research scientists, to build molecules with the program. Thanks to the Drawing tool, users can click to add elements after defining the number and type of bonds. The fragments library (Figure 2) has numerous frequently used chemical compounds, thus removing the need for the user to piece them together themselves.

In navigation mode, you can view from all sides the molecules you have built. Compounds can be rotated in all three dimensions, and a zoom feature lets you view the details. A tool for automatic optimization is based on various chemical force fields such as MMFF (Merck Molecular Force Field) and UFF (Universal Force Field).

One of Avogadro's strengths is its modular structure, which supports plugin extensions. Developers can add their own 3D rendering functions

Ilja Mašík, Fotolia

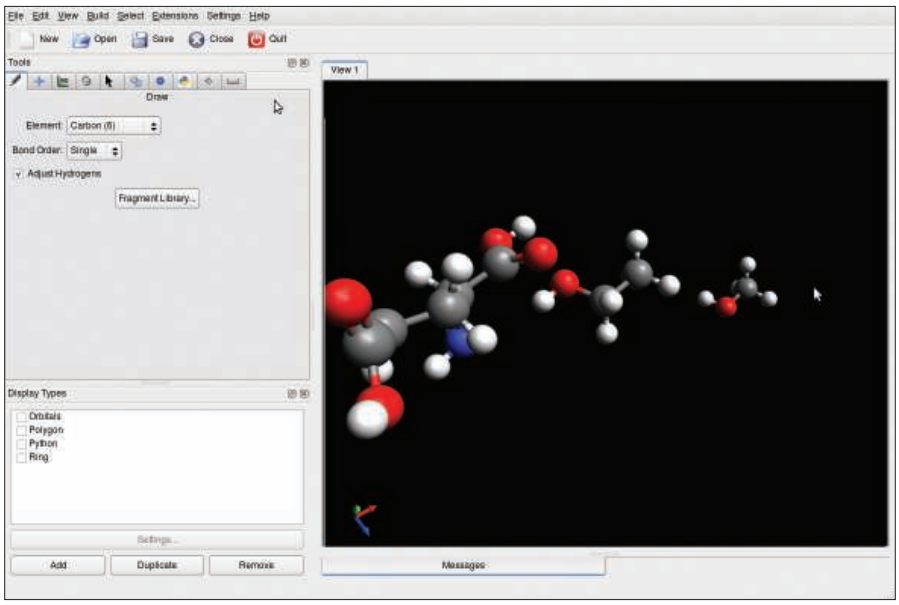

Figure 1: In Avogadro, users can click their way through molecular structures they have built themselves. The 3D renderer makes easy work of resizing and rotating.

and define their own tools and commands. The interface to the multi-talented Open Babel [3] ensures compatibility with numerous other chemistry programs.

Open Babel, a hybrid of programs designed for end users and a toolkit for programmers, was derived from Babel's format conversion tool. It translates, detects, and converts more than 90 typical file formats used in the field of chemistry. The applications in the package help the user modify and translate them.

Many free projects in the chemistry field rely on the programming library. Specialist tools for biochemistry and organic and inorganic chemistry make Open Babel an attractive starting point for developers.

New Beginnings

The structure of version 0.9 aims to be as close to the final release as possible. This explains why the developers rewrote many sections of the code. In the process, they implemented numerous

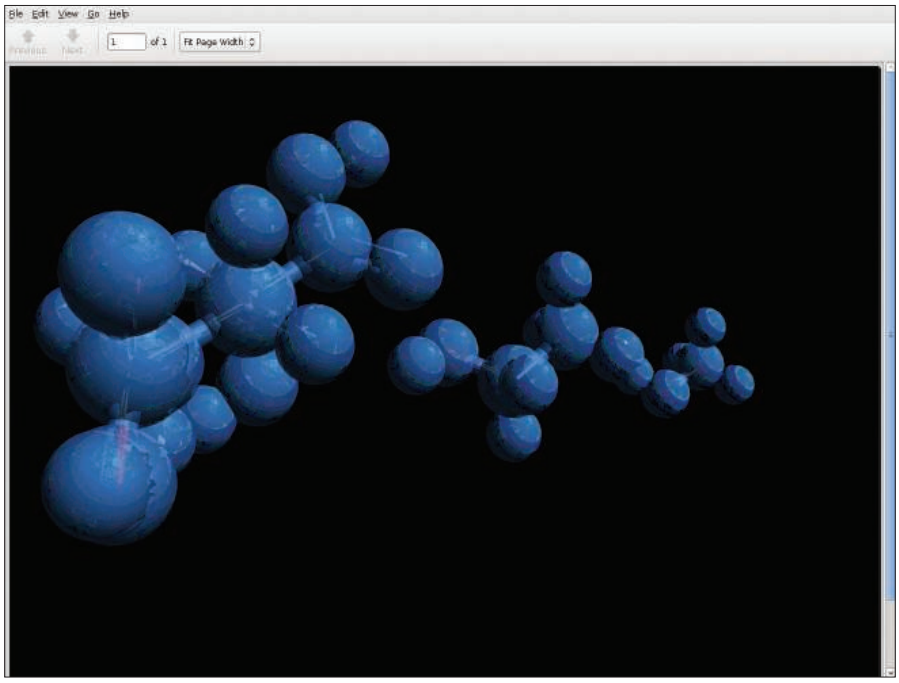

Figure 3: The integrated renderer creates all popular image formats, including vector graphics, which scale without loss. Avogadro also relies on POV-Ray.

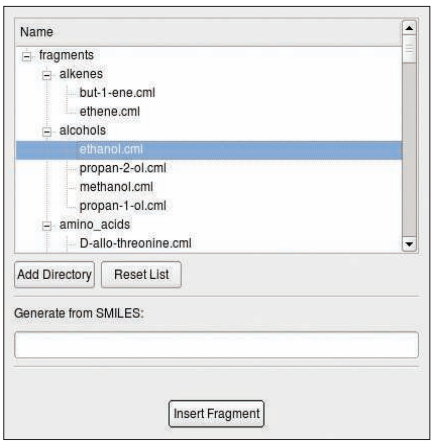

Figure 2: Numerous prebuilt molecular fragments help users get started quickly. Virtual ethanol is not suitable for drinking!

new features, including an interface to the POV-Ray [4] 3D modeling program. It lets you use this external utility to export three-dimensional creations as PNG graphics. The internal 3D renderer can create all popular image formats, including vector graphics (Figure 3), which have the advantage of being scalable without degrading image quality.

Conclusion

The homepage features the Avogadro developers' roadmap, which they intend to complete for the final release. One of the major items on the list is documentation and translation. Besides the English language version, translations for French and German exist, although they are not complete. The program still lacks an integrated help system; the menu simply features links to the documentation pages on the project homepage. Unfortunately, many user questions still remain unanswered.

The developers are also looking to clean up the interface because the newly implemented functions have affected its clarity. They also plan a plugin manager to make it easier for users to enable and disable plugins. Many other plans give rise to hope that the final release will be a very solid piece of software. ■

INFO

[1] Avogadro: *http://avogadro.openmolecules.net*

[2] Marcus D. Hanwell's blog: *http://blog.cryos.net*

[3] Open Babel: *http://openbabel.org*

[4] POV-Ray: *http://www.povray.org*