

The Monthly GNU Column

BRAVE GNU WORLD

This column looks into projects and current affairs in the world of free software from the perspective of the GNU Project and the FSF. In this issue, I'll focus on Comspari and the EU decision on software patents. **BY GEORG**

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Proprietary software is ill-suited for scientific research because closed data formats and unknown algorithms leave no scope for validation. Free software is a better option, as the Comspari tool demonstrates.

Comspari

Scientists regularly face the challenge of having to compare two samples with only minimal difference in quality. Extremely small deviations in spectra are extremely difficult to detect by computational means. Graphs give scientists a far more practical approach, allowing them to pinpoint slight differences in complex records quickly and intuitively. Comspari [1], a free software application that prepares spectral data for comparison, is rapidly gaining popularity as a

tool to assist with tasks such as mass spectrometry.

The name *Comspari* is short for Comparison of Spectral and Retention Information. Comspari was developed in C and uses Gnuplot [2] to render graphs. The program is quite widespread in scientific circles and supports a number of different platforms. Comspari runs in any operating system supported by Gnuplot, including Linux and other Unix variants, as well as OS/2, Mac OS, and Microsoft Windows.

Jonathan Katz and Jörg Hau, the Comspari authors, made their project available to the general public as free software under the General Public License (GPL). Additionally, the authors published the project in cooperation

with D. S. Dumlao and S. Clarke in the "Journal of the American Society for Mass Spectrometry". The paper, which is entitled, "A New Technique (COMSPARI) to Facilitate the Identification of Minor Compounds in Complex Mixtures by GC/MS and LC/MS: Tools for the Visualisation of Matched Datasets," is available online at [3].

Issues

The issues causing John and Jörg the biggest headaches are a lack of time and faulty data files. Both developers are full-time industrial research scientists. Jörg argues that the effort he puts into the software pays back due to the amount of time he saves in his research work. But this often leads to him only implement-

Comments & Suggestions

The email address column@brave-gnu-world.org is available for your comments on and suggestions to Brave GNU World. The GNU project homepage is at <http://www.gnu.org>. Georg's "Brave GNU World" column is available online at <http://brave-gnu-world.org> and the "We run GNU" initiative has a website at: <http://www.gnu.org/brave-gnu-world/rungnu/rungnu.de.html>



Figure 1: Opponents of software patents are pinning their hopes on the European Parliament. Representatives are debating the second reading of the bill.

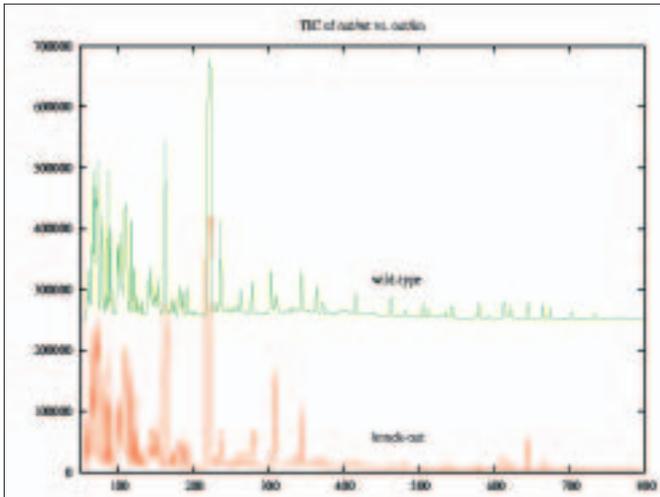


Figure 2: Gnuplot helps Comspari to convert the data acquired by mass spectrometry experiments into intuitive graphs.

ing the things he really needs for his current experiments.

Trouble with unusable data files makes one fundamental problem quite clear. Use of open formats is a major prerequisite for working with scientific records. This is what the Net-CDF standard gives scientists in principle, but in practical applications, manufacturers of mass spectrometers tend to use proprietary formats for a variety of reasons. This forces scientists to trust the manufacturer's evaluation software unquestioningly without being able to validate the results of their own or third-party experiments. In other words, one of the basic conditions for scientific work is not fulfilled.

Additionally, proprietary software makes it far more difficult to investigate topics not envisaged by the manufacturer. In other words, manufacturers more or less dictate the fields that laboratories can investigate. Faced with pressure from scientists, some manufacturers provide conversion tools to convert proprietary data to Net-CDF format. Unfortunately, their implementations of this open standard are often poor, and this can lead to evaluation problems. Comspari uses the free `cdfread` [4] software tool written by Jörg to parse this kind of file.

The current focus of the Comspari project is on improved error handling and correcting. But migrating the file format from ASCII to a compressed format would also make sense, based on the volume of data to be processed. John and Jörg also need more support from

hardware manufacturers to resolve occasional conversion issues.

There are no end of opportunities for volunteers to lend a hand; John and Jörg are both looking for volunteers to write documentation. Although many functions are self-explanatory. A graphical user interface is another item on the to-do list for

similar reasons. If you are interested, check out the homepage at [1].

Software Patents

March 7 2005 was one of the blackest days on record for supporters of free software in Europe. Against the will of the European Parliament and many national parliaments, and against the official requests by many countries to open further discussions, the EU Council of Ministers officially sanctioned the introduction of software patents and passed the paper to the European Parliament for a second reading.

These actions give rise to the question of whether the rules required the Council to pass this bill in order to comply with formalities, as the EU Council president maintains. Or could it be that the president is simply wiping the floor with democracy? The parliament has already commented twice: first, with a clear rebuttal of patents on logic, and secondly with a firm request for a relaunch of the directive. The Council ignored both requests.

If the parliament wants to avoid admitting its own impotence, it has no alternative but to flex its muscles. By accepting the guidelines, the parliament would seriously compromise its own influence on European politics.

Other Matters

The stir caused by the software patent issue has meant that other important topics are slipping out of the public focus. For example, the media is paying little attention to negotiations between

the European Commission and Microsoft at the European Court of Justice [5] or to the state of affairs within the United Nations Working Group on Internet Governance (WGIG), which has the task of laying down the structures for possible Internet governance.

The papers presented by the WGIG working group were a disaster [6]. Even former ICANN directors such as Karl Auerbach were fairly open in their criticism of this group. Most of them seem to be unaware of the existence of the World Intellectual Property Organization (WIPO, [7]) although it is to be reformed. This said, the organization is responsible for the management of the Trips agreement, which relates to intellectual property in international trade and is thus tangled with the US DMCA and EUCD – notorious laws banning the creation of copies for private use. More people should be involved with these processes and work together in a more coordinated way. The Free Software Foundation Europe has set up a Fellowship [8] to provide donors with more immediate access to information on the legal affairs surrounding free software. ■

INFO

- [1] Comspari Homepage: <http://www.biomechanic.org/comspari/>
- [2] Gnuplot: <http://www.gnuplot.info>
- [3] J. E. Katz, J. Hau, D. S. Dumlao and S. Clarke, "A New Technique (COMSPARI) to Facilitate the Identification of Minor Compounds in Complex Mixtures by GC/MS and LC/MS: Tools for the Visualisation of Matched Datasets": *J. Amer. Soc. Mass Spectrom.* 15 (2004), 580-584, <http://dx.doi.org/10.1016/j.jasms.2003.12.011>
- [4] `Cdfread`: <http://homepage.sunrise.ch/mysunrise/joerg.hau/sci/index.htm#cdfread>
- [5] FSFE, Microsoft versus Samba: <http://www.germany.fsfeurope.org/projects/ms-vs-eu/ms-vs-eu.en.html>
- [6] FSFE, Working Group on Internet Governance: <http://www.germany.fsfeurope.org/projects/wsis/wsis.en.html>
- [7] FSFE, WIPO Page: <http://www.germany.fsfeurope.org/projects/wipo/wipo.en.html>
- [8] FSFE Fellowship: <http://www.fsfe.org>
- [9] Free Software Foundation Europe (FSFE): <http://fsfeurope.org>
- [10] GnuPG: <http://www.gnupg.org>