Analytical computing survey

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ith preparations for Analytical Laboratory Informatics 2004 in London running at full tilt I have decided to use this column to carry out a survey of computer use in the analytical laboratory. We last carried out such a survey way back in 1998[1] during the European Congress on Molecular Spectroscopy (EUCMOS) in Prague, so six years is a good time to repeat the exercise and will provide us all with a basis for discussions during ALI2004 at the end of June.

Even if you are not attending the discussions during the conference I would like to ask you to take a couple of minutes to fill out the short form on the ALI website – or download the PDF version and fax it though to us at the number shown – as the more responses we get, the more representative the answers will be and the greater the likelihood that any strategic changes in direction wished by the Analytical Informatics community from their vendors will actually be carried through!

In this way we hope to enable non-attendees to also influence developments and discussions, so please feel free to add as much additional comments as you want!

Survey format

The anonymous survey is divided into short sections on operating systems, typical analytical software use and future plans/wishes/needs.

Operating systems

In 1998, there was a choice between the Windows, Unix, OS2 and MacOS operating systems, and the distribution can be seen in Figure 1. Looking at our laboratories, this choice has been somewhat simplified in recent years but the question will reflect the previous survey to keep the statistics going.

In 1998, this reflected a 90% dominance of personal computers in the laboratory and it was predicted that the relatively high percentage of OS2 users would diminish in the future as the major instrument vendor who was rolling out instrument control software on OS2 was at that stage switching to Microsoft Windows.

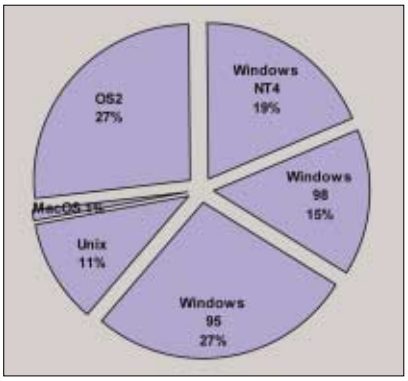

Figure 1. Distribution of laboratory PC operating system use reported during EUCMOS in 1998.

Analytical software

The picture reported in 1998 for analytical software use would seem with hindsight to be somewhat slanted by the particular audience attending the EUCMOS meeting. Furthermore, at the time of conducting the survey the instrument manufacturers software used for additional data processing off-instrument had been ignored and so the particular answers shown in Figure 2 probably are not too representative of general analytical software usage.

In recent years, the instrument vendors have started to include more functionality in their packages so that more data analysis is probably now possible than ever before. This will be reflected in the modified questions in this year's survey.

Plans/wishes/needs

In this section we aim to harvest information which will be of use to all solution providers in our market place. In the past, we identified, during the discussion session, specific needs amongst our community. In 1998 there was general dissatisfaction with the software that was available as well as a feeling that the users had no possibility of changing the situation! Rather depressing really!

Although there was much made during the plenary lectures about the availability of standards, the users still expressed the need for better interoperability between software packages from different vendors and even between different packages from the same vendor. I hope that in six years things have improved.

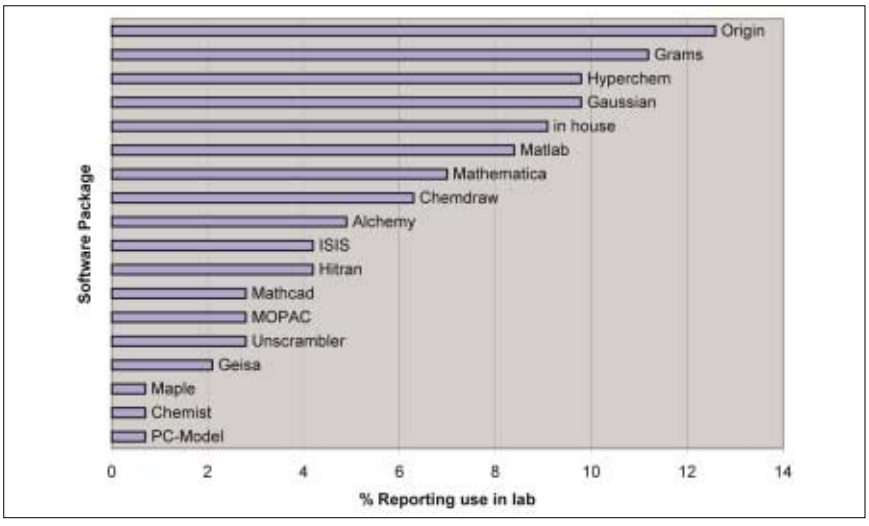

Figure 2. Software packages reported as being in use in the 1998 survey.

In some communities it is commonplace now for instrument control codes to be exchanged between competing vendors allowing instruments from manufacturer A to be run from the control software of manufacturer B or third party software house C.

Against this, the two LECIS standards (Laboratory Equipment Control Interface Specification) for a common instrument interface protocol, LECIS 1 an ASTM standard[2] and LECIS 2 from the OMG[3] have not been widely adopted by the mainstream instrument manufacturers.

Back in 1998 more advanced chemometric tools were being made available as standard in spectrometer control packages. This had, however, raised fears that the inherent dangers of over-fitting data were not being sufficiently addressed in order to help inexperienced spectroscopists handle the additional computing power that was becoming available. I must admit that the work of my co-column Editor in pushing for "Good Chemometrics Practice" has hopefully raised awareness in the community of the potential pitfalls in using these packages without due consideration, but I personally have not been aware of clear unambiguous automated warnings starting to appear when data was being over-fitted.

Since 1998, of course, developments in the regulatory area have dominated a lot of the purchasing pressure being brought by users such as the FDA electronic records and electronic signatures rule 21 CFR part 11, and more recently the EPA equivalent CROMERRR.

This has fortunately tended to provide corporate political and upper management backing for initiatives in modern Archiving Strategies. The problematic introduction of early Electronic Lab. Notebooks and the newer generation of integrated informatics solutions can only be regarded as a very positive outcome of what is essentially end-user pressure.

High-throughput techniques have greatly increased the availability of data which the analytical spectroscopists should be analysing, but are we able to master this extra burden with the Informatics tools that are currently available?

A.M.C. Davies highlighted the PAT initiative in the last edition of *Spectroscopy Europe* so I don't need to go into the importance of what this could mean again here.[4]

Finally, the survey wants to establish your attitudes to the availability and usefulness of Public Reference Data.

Summary

Even if you cannot join us at the Heathrow Sheraton for the conference I am very keen that readers of this column, who have been very supportive over the years, have their views registered during the meeting so please follow the web link below to the *Spectroscopy Europe* Readers' Survey page on the ALI web site and sacrifice a few minutes to make your views known.

http://www.ali2004.org

Alternatively, you could download, print out and fax back the PDF version of the survey available at the same website. For readers not attending the meeting we will publish the results of the survey after the summer holidays.

References

1. A.N. Davies, *Spectrosc. Europe* **10(5),** 22–24 (1998).
2. *LECIS 1*. The official ASTM E1998-98 LECIS standard document: www.astm.org.
3. www.lecis.org/documents/CORBA%20LECIS%2002-09-13.pdf
4. A.M.C. Davies, *Spectrosc. Europe* **16(2),** 33–34 (2004).