Software Fayre

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Throughout the entire IUCr Glasgow Congress, a Software Fayre was held to allow both software authors and users to interact with the various freely available packages useful to Crystallographers. Thanks to the generosity and helpfulness of the organising committee, SGI and Compaq; especially Chris Gilmore, Stuart Mackay and David Thom, the Fayre had access to 3 Silicon Graphics O2s, 2 Compaq PCs running Redhat Linux and 5 Compaq PCs running Window95; as well as an overhead computer projector for demonstrating software to larger crowds. The computers could not be connected to the internet to enable download of software and patches, thus software was installed off CD-ROMs. As the long queue on the Internet Cafe turned many a calm crystallographer into a rampaging desperado needing an internet fix; the lack of internet access for the Software Fayre computers actually allowed a wide range of crystallographic software to be demonstrated.

Small Molecule Single Crystal Software:

A healthy variety of available small molecule single crystal solution and refinement software was presented at the Fayre. These include: John Gallager demonstrating the ORTEX for Windows single crystal suite (based around Shelx for solution and refinement)(1); Syd Hall and Brian Skelton, the XTAL single crystal solution and refinement suite running on UNIX and Windows(2); Paul Mallinson and Thomas Richter, the “Project XD” Charge Density Software(3); David Watkin and Richard Cooper the new GUI based CRYSTALS refinement suite for Windows(4); Louis Farrugia the WinGX for Windows suite (based around Shelxs, Sir and Dirdif for solution and Shelxl for refinement)(5). Riccardo Spagna demonstrated the combination of using Sir and CAOS (Crystal Analysis Operating System)(6) to solve (Sir for direct methods(7), CAOS for Patterson methods) and CAOS for refining structures; Michal Dusek, the JANA98 program (UNIX and PC) for refinement of ordinary and modulated structures(8); Paul and Gezina Beurskens the Patterson methods and difference direct methods based DIRDIF structure solution package (UNIC and PC) (9). Rene de Gelder showed how easy it is to compile and install the the direct methods CRUNCH structure solution package under UNIX and Linux(10) for handling difficult structures. Frantisek Pavelcik demonstrated the Patterson methods based XFPA structure solution program (UNIX and PC) (11) and Ton Spek the Platon/”System S” single crystal suite (UNIX/Linux) (Shelxs, Sir, Dirdif and Crunch for structure solution, Shelxl for refinement and powerful Platon tools)(12).

Powder Diffraction

Powder diffraction software demonstrations included: Robin Shirley on the CRYSFIRE powder indexing suite(13) who successfully indexed of some Protein powder diffraction data provided by Bob von Dreele; Armel Le Bail on solving structures from powder diffraction data using the Monte Carlo based methods incorporated into the ESPOIR software(14); and Juan Rodriguez-Carvajal showed the latest Fullprof Rietveld friendly plugin, the “GFOURIER” Fourier Map generation and display software(15). A variety of other powder diffraction software was available for people to try out.

Protein/Macromolecular Crystallography:

On the protein side, software demonstrations included Pamela Williams on the XtalView program for UNIX (fitting electron density maps and solving structures by MIR and MAD software); Isabel Uzon applying Shelxpro/Shelxl for refinement of protein structures(17) (with the possibility of using XtalView

to view the maps (16)); Marian Szebenyi, the MacCHESS Software/GUI for processing protein crystallographic data using DPS programs, mosflm, and some CCP4 programs(18); and a demonstration of MICE (Molecular Sciences and Interaction Environments)(19). Bob von Dreele also showed GSAS in action which is now also used powder diffraction refinement of Protein structures(20), with maps and structure linking into the Swiss-PDB Viewer(21).

Databases, Structure Manipulation, Diffuse Scattering and Educational Software:

Alan Hewat used one of the SGI O2s to demonstrate the web based ICSD (Inorganic Crystal Structure Database)(22) and a Linux machine was applied for a DISCUS diffuse scattering/ crystallographic teaching demonstration by Thomas Proffen and Reinhard Neder(23). PowderCell for Windows(24) and Cryscon for Windows(25) were shown as effective tools for dealing with structure transformations, including classical phase transformations.

Misc Things:

Prize for most impressive demonstration goes to a presently anonymous 10 to 12 year old accompanying person who managed to successfully hack one of the SGI O2 IRIX machines in around 30 to 60 seconds (the approximate time I had my back turned) and figured out how to get the “Doom” game (26) into action. An psuedo-formal booking on computer security ended up as small impromptu demonstrations on securing crystallographic servers; and it was interesting to learn of the wide range of crystallographic UNIX computers that been successfully compromised and burgled by hackers(insecure installations of Linux being the main culprit). Pages on installing dual boot Windows/secure Redhat Linux(27) combinations and the more secure FreeBSD(28) based UNIX operating system for Crystallographic information serving are available on the CCP14 website(29).

Lessons learnt from the Fayre for anyone interested in organising any such events in the future include: due to the extremely busy conference schedule, multiple bookings by software authors is more effective than just single bookings; if internet access is possible, it is important to have “lockable” Internet links to restrict inappropriate use; Computer Fayres are best located as close as possible to the Poster area (as many of the programs were described or mentioned on the posters); to enabled maximum flexibility for installing software and enabling demonstrations of network based applications, creating a local intranet connecting the software Fayre computers is highly desirable.

Most of the above mentioned software is available for download via the internet for anyone to try out. The powder diffraction and single crystal software is also mirrored (where possible) on the CCP14 website and its mirrors (http://www.ccp14.ac.uk). Thus there is no excuse not to try some of these tools and check their suitability to assist in high quality crystallographic analysis.

1. ORTEX for Windows Single Crystal Suite (http://www.nuigalway.ie/cryst/)
2. XTAL (Windows/UNIX) Single Crystal Suite (http://www.crystal.uwa.edu.au/Crystal/xtal/)
3. Project XD Charge Density Software (http://www.chem.gla.ac.uk/~paul/xd.html)
4. CRYSTALS for Windows Single Crystal Suite (http://www.xtl.ox.ac.uk/crystals.html)
5. WinGX for Windows Single Crystal Suite (http://www.chem.gla.ac.uk/~louis/software/)
6. CAOS (Windows/UNIX)Single Crystal Suite (http://www.isc.mlib.cnr.it/caos/)
7. Sir Sirware (Sir97 - Windows/UNIX) Structure Solution (http://www.ba.cnr.it/IRMEC/SirWare_main.html)
8. JANA ordinary and modulated Structure Refinement Suite (http://www-xray.fzu.cz/jana/jana.html)
9. DIRDIF Structure Solution (http://www-xtal.sci.kun.nl/xtal/documents/software/dirdif.html)

10. CRUNCH Structure Solution (http://www.ccp14.ac.uk/ccp/web-mirrors/dirdif/xtal/documents/software/crunch.html)
11. XFPA Structure Solution (at time of writing no website but check http://www.ccp14.ac.uk/mirror)
12. Platon/"System S" (http://www.cryst.chem.uu.nl/platon/)
13. CRYSFIRE Powder Indexing Suite (http://www.ccp14.ac.uk/tutorial/crys/)
14. ESPOIR Monte Carlo Structure Solution (http://www.cristal.org/sdpd/espoir/)
15. Fullprof Rietveld and Single Crystal Software (ftp://charybde.saclay.cea.fr/pub/divers/)
16. XTALVIEW MIR, MAD, real-space / direct-space refinement software (http://www.scripps.edu/pub/dem-web/)
17. Shelx Structure Solution and Refinement software(http://shelx.uni-ac.gwdg.de/SHELX/)
18. MacCHESS (http://www.chess.cornell.edu/MacCHESS/)
19. MICE (Molecular Sciences and Interaction Environments) (http://MICE.sdsc.edu/)
20. GSAS (General Structure Analysis System) (ftp://ftp.lanl.gov/public/gsas/)
21. Swiss-PDB Viewer (http://www.expasy.ch/spdbv/mainpage.html)
22. Web based ICSD (Inorganic Crystal Structure Database) (http://barns.ill.fr/dif/icsd/)
23. DISCUS - "DIffuse SCattering and defect strUcture Simulation" (http://www.pa.msu.edu/~proffen/discus/discus.html)
24. Powder Cell for Windows (http://www.bam.de/a_v/v_1/powder/e_cell.html)
25. Cryscon (http://www.shapesoftware.com/#anchor_cryscon)
26. IDSoftware (Quake, Doom) (http://www.idsoftware.com)
27. Redhat Linux (http://www.redhat.com)
28. FreeBSD UNIX for PCs (http://www.freebsd.org)
29. For CCP14 Windows/Linux and Windows/BSD dual boot pages, refer http://www.ccp14.ac.uk/solution/

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