10. Facilities

Computing

R. K. Bryan

Central Servers

The following systems provide central file serving and backup services which are available to all systems on the laboratory network:

- A high-availability Linux fileserver cluster, comprising:
  - two Compaq Proliant ML370 G2 systems, running Suse Linux and Mission Critical Linux Convolo.
  - Jetstor III Raid array - six Seagate 180GB disks, 900GB useable space, dual Ultra160 SCSI interface. This may be served by either system.
  - Compaq MLS5026 SuperDLT robot. 100GB/tape. Data transfer speed up to 70Gb/hr. Magazine capacity 25 tapes.
  - GForce RI Raid array with eight Maxtor 200GB disks, 1.2TB useable space. Due to some continuing reliability problems, an alternative stand-alone system is currently being used to serve this storage, to avoid periodic reboots of the main systems.
- A VMS cluster consisting of an AlphaServer 1200 and AlphaStation 500, providing access to about 800GB of RAID disk storage, with a TL891 DLT tape robot. The storage is served to the rest of the laboratory systems using various network protocols (VMScluster, NFS, SMB and AppleTalk). This also runs network services for mail, POP, IMAP2, IMAP4, DHCP and the laboratory web server. The inherent security of the VMS architecture gives greater protection against potential external disruption to these services. The operating system version was upgraded to 7.3-1, which provides improved TCP/IP support, and the Samba software (for file and print services to Windows systems) was updated.
- A 4-processor Compaq AlphaServer 4100 running Compaq Unix, which serves about 50GB of storage, and acts as the NIS master node.
- In addition, two Beowulf PC clusters provide a high-performance computing resource. The first, installed in 2001 for Mark Sansom's group, consists of 32 dual 750 MHZ PIII nodes, and the second, a joint resource for the Sansom, Noble and Garman groups which was installed in 2003, consists of 67 dual 2.4GHz PIV nodes, and also 1.8TB of local RAID storage.

In general, all these systems have run reliably, with uptimes of many months. Disappointingly, the economical RAID arrays using IDE disks have not proved as reliable as their predecessors using SCSI disks, although different brands and models of disks seem to vary greatly in this respect.

Laboratory Network

The laboratory network continues to be based on a 100Mbit/sec Fast Ethernet network, plus a Gigabit switch in the computer room which provides a higher-speed connection to several of the central systems. This network is connected *via* a Firewall (Intel PC running BSD Unix and pf packet filter) to the University 10GB backbone ethernet, which provides access both to other units within the University and to the external Internet connection.

Part of Mark Sansom's group 'decanted' to the Biochemistry building in the Autumn of 2003, and of course it was important that they continued to access the laboratory servers transparently, and in particular the NIS and NFS services which are protected against external access. This required a certain amount of reconfiguration of our firewall, and for the Biochemistry Network Manager to make corresponding changes to their firewall, plus a small amount of retuning due to higher throughput.

About 200 host addresses are registered on the Laboratory network, which include a wide variety of systems:- the central servers as described above; a large number of desktop systems, including Intel systems running either Windows or Linux, and Apple Macintosh computers; personal laptop computers; and a number of systems dedicated to specific tasks, such as control of the X-ray Area Detectors and EM Image aquisition.

X-ray Facilities

Ed Lowe and Elspeth Garman

In July 2003 we tendered for a new microfocus X-ray generator funded largely by the Wellcome Trust but also with help from the Equipment Fund of the University of Oxford. The Bruker MicroStar was ordered on 20/12/03 and installed in T3 on 8/6/04. The generator was supplied with Montel optics on both the left and right ports. X-rays were produced on 9/6/04, less than 24 hours after the beginning of the installation.

The new generator has a maximum operating power of 2.7 kW. Measurements carried out by Robin Owen using a photodiode calibrated at the ESRF indicate a photon flux at 80% maximum power (40kV / 55mA) of 7.24×10^8 photons s^{-1}, almost 3-fold higher than the 2.5×10^8 photons s^{-1} measured for the RU200H in T5 operating at maximum power. The attached Montel multilayer optics produce a beam of cross section $150 \times 150\ \mu m^2$ at the sample. This small beam size in combination with the higher flux noted above should now facilitate the in-house study of the increasing number of small crystal samples which we are obtaining from robot crystallisation trials.

The RU200H generator (`Myrtle') with a Mar345 imaging plate detector and Osmic Optics in T5 ran very smoothly this year. The anode annual rebuild was carried out by us on August 5th without incident. Users included numerous members of the LMB and OCMS, and Dr. Arzhang Ardavan's correlated electron systems group from the Clarendon Laboratory collaborating with Robin Owen and Elspeth Garman to investigate the effects of radiation damage on organic superconductors.

The RU200H in T3, which had been used since 1991 and run for around 76,685 hours, was decommissioned in April 2004 by Rigaku/MSC engineers. It was donated to the National University of Mexico in Cuernavaca, and will be reinstalled there. The removal and transportation were carried out by Inport Export Services of Bristol, who were extremely efficient and professional. To obtain a Safety Certificate of Compliance prior to donation, the generator had to run for 15 minutes at full power (60kV and 90mA) before being dismantled. It is a tribute to the robust technology of rotating anode generators that this was achieved after 12 years of running.

The false floor in T3 was then removed and a new lino floor fitted with up the wall coving to give the room Biological category 2 status and allow diffraction experiments on virus crystals in the future.

Postscript

The Dunn School of Pathology decommissioned their X-ray equipment in November 2004 and kindly donated their Mar345 Imaging plate detector (plus their 600 series Oxford Cryostream and blue Osmic mirrors) to us. We have installed the detector on the right side of the MicroStar, and are thus leaving the T5 facility in tact for the moment.

Crystallisation facility

Marc Morgan and Jenny Gibson

The Oxford LMB crystallisation facility currently has over 40 users and this number is growing due to the acquisition of new technologies designed to improve result throughput and scoring. In late 2002 the LMB purchased a TECAN liquid handling platform with the aim of fully automating the setup of macromolecular crystallisation trials. It was at first necessary to reconfigure the liquid handling system for crystallographic use. Since then the TECAN Genesis 150 has been operating effectively in its new role. We will briefly outline the set-up, level and mode of use. In October 2003, the LMB also acquired a high definition Leica microscope with an automated Prior stage in order to keep pace with the results produced by the robot.

The reconfigured TECAN robot has a unique set-up that allows it to reproducibly pipette a variety of crystallisation screens. The liquid handling arm has a total of 8 tips: 4 standard volume tips, which pipette volumes between 250 μl and 0.5μl, and 4 low volume tips which pipette volumes between 1 and 0.25 μl. The standard tips are powered by 250 μl capacity syringes, and the low volume tips are powered by smaller 50 μl NPS (Nano-Pipetting System) syringes.

The original design of 50 μl syringes was identical to that of the larger 250 μl syringes: a glass chamber fitted with a Teflon capped aluminium syringe plunger. However, after several months of use, substantial wear and tear on the 50 μl syringes was noticed, which in turn significantly impaired the accuracy and reproducibility of low-volume pipetting. In consultation with TECAN the glass-clad aluminium plungers were replaced with more durable ceramic plungers enclosed in a plastic syringe body. These have been a great success and have certainly proved flexible enough to cope with the demands placed on the system.

Before leaving the LMB on his retirement Mike Pritchard was involved in the creation of a new rack for the robot, allowing samples to be pipetted directly from 48 x 1.5 ml micro tubes and kept on ice if necessary. This enables robot users to explore their crystallisation conditions further using various additive screens. Planned future developments for the robot include new anti-evaporation covers, and further programming to give users greater scope in setting up secondary crystallisation trials.

The automated Leica microscope is now fully operational. Users of the microscope can either scan an entire 96 well crystallisation plate, or select an individual well for imaging. Picture quality and the speed of data processing are both highly satisfactory, with the system able to generate 96 high definition images in under

5 minutes. The lens depth of field is good enough to see the majority of crystalline particulates at the low magnifications required for plate scanning, but also performs excellently at the high magnifications required for more in-depth analysis. It has also been effective in overcoming problems of imaging at very low exposures necessary for viewing light-sensitive proteins. Planned future developments for the microscope include an image/crystallisation database for cataloguing interesting crystallisation characteristics. We are also continually testing new crystallisation plates for improved picture quality, although the images obtained with the current plates are highly satisfactory.

Other developments in the crystallisation facility include the operation of the Tecan SpectraFluor Plus, a fully automatic fluorimeter for measuring samples on a microplate. The Tecan robot is configured to pipette reagents on microplates, which can then be read on the fluorimeter. We also set up the S9 website which has proved a very useful tool for users of the facility (www.biop.ox.ac.uk/S9).

The crystallisation facility boasts an ever-growing number of users, who are now profiting from the new technologies recently installed. The addition of the robot has increased not only throughput, but also output. The full impact of the microscope will become apparent once the crystallisation database is operational.