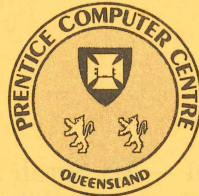


# PRENTICE COMPUTER CENTRE

UNIVERSITY OF QUEENSLAND, ST. LUCIA, QUEENSLAND, AUSTRALIA. 4067.



## NEWSLETTER

N-314

August 1987

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Authorized by the Director of the Computer Centre

## Phone Numbers for Enquiries

External users may dial direct by prefixing these extension numbers with 377.

<b>Management</b>	<b>Extension</b>
Director – Mr Alan Coulter	2189
Deputy Director – Mr John Noad	3017
Manager, Applications Development – Ms Sarah Barry	4281
Manager, Central Computing Facilities – Mr Allan Woodland	4017
Manager, Distributed Computing – Mr Anthony Bird	3391
Manager, Engineering and Communications Services – Mr Graham Rees	3288
Manager, Finance and Administration – Mr Denis Antonellie	3963
Manager, Operations – Mr Ian Armstrong	3471
Manager, User Liaison – Mr Geoffrey Dengate	3944

### Principal Service Centres

Personal Computer Support Group – Mr Chris Barker	4233
Contract Programming & Feasibility Studies – Ms Sarah Barry	4281
System Status Automatic Answering	3101
General Enquiries & Course Enrolments	3018
Dial-up moden numbers	(300 bps) 377 2977
	(1200 bps) 377 2922
	(1200/75 bps) 377 2655

<b>Service Advice &amp; Problem Reporting</b>	<b>Mail Box</b>	<b>Extension</b>
Central Services HELP Desk (0830–1630)	CCHELP	3025
Program Librarian – Mr David Molloy		3025
PC Repairs and Maintenance		3938*
Hardware Fault Reporting		3938*
Accounts (0830–1630) – Ms Lyndal Hill		2188
Operations		3212
Data Entry – Ms Ngaire Brown		3967

### Engineering and Maintenance

Development and Communications	ENGIN	4307
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### Griffith University

External users may dial direct by prefixing these extension numbers with 275.

Consulting	7796
Computer Services	7560
Computing Co-ordinator	7561

\*NOTE: After 4.45 pm and at weekends, X3938 is serviced by a message recorder. Users wishing to report PC, terminal, communications and other hardware faults can leave their name, number and fault details.

## 1. Newsletter Summary

- CLUSTAN is a widely used cluster analysis package which helps to solve classification problems over a diverse range of applications. It is now available for use on the IBM 3083 system.
- CHEM-X, a molecular modelling package is available on the VAX 11/780.
- VAX users can now print documents on A4 sheets on the high quality IBM 6670 laser printer using the new LPRINT command.
- Macintosh Personal Computers are now available for hire in addition to IBM XT systems.
- Macintosh users who wish to include equations in documents written with Macintosh word processing programs will be interested in MacEqn. The PCC has a licence and can demonstrate this facility.
- Apologies are provided for the difficulties caused by the unannounced upgrade to the MICOM circuit switch. Additional facilities provided are described.
- Details of PC and mainframe courses are provided.

*Director  
ext. 2189*

## 2. Central Computing Facilities – Allan Woodland, ext. 4017

### 2.1 Cluster Analysis Package on UQVM

Version 3.2 of the Cluster Analysis package CLUSTAN is now available on UQVM (IBM 3083).

Cluster Analysis is an exploratory method to help solve classification problems. Clustan can be used to reveal associations and structure in data with the results contributing to the development of a classification scheme.

Applications which have used cluster analysis are listed below to illustrate the diverse range of the subject:-

- Puberty rites of American Indian tribes
- Tribal classifications of Australian Aborigines
- National voting patterns at the UN
- Housing types by their furniture stocks
- Impact craters and volcanoes on earth, moon and Mars
- Wild plant communities and agricultural crops
- Evolutionary processes in biological taxonomy
- Influenza viruses by antigenetic relationships
- Urban speech varieties from a linguistic survey
- Heroic, comic and gender patterns in literary fantasy
- Job classes and personnel functions
- Data base relationships in management information systems

Clustan can be used interactively or non-interactively. For more information, enter **CLUSTAN ?** or **INFO CLUSTAN**.

## References

CLUSTAN Command Language for CLUSTAN Version 3.2.

This is available on-line; to obtain a listing, enter:

**PRINT CLUSTAN LISTING X**

CLUSTAN User Manual and Supplement for Version 2.1.

Wilfred Brimblecombe  
extension 4287

## 2.2 CHEM-X : A Molecular Modelling Package

CHEM-X is a suite of molecular modelling programs, useful for chemists and others interested in looking at the structure of organic, inorganic, protein and peptide molecules.

This is now available for use on the VAX 11/780.

The programs comprise:

- CHEMCORE – the main program unit. The molecule of interest must first be specified by input of some atomic coordinates. The formats are various (see reference manual). Further options:
  - ★ Display structure in skeleton, ball and stick or space-filled form, with modifications to scale, colour, etc.
  - ★ Geometry calculations from simple distances and angles, to distances from planes, torsional angles.
  - ★ Energy calculations, e.g. to predict bond lengths, torsional angles, influence of inter-molecular forces.
  - ★ Van De Waals
  - ★ Molecular mechanics
  - ★ Geometry optimisation
  - ★ Hydrogen bonding
- CHEMMODEL — conformational and spatial analysis, e.g. spherical dotted surfaces, dummy atom cages, Connolly surfaces, contour maps.
- CHEMMOVIE — display for high resolution devices only.
- CHEMQM — Quantum Mechanical calculations, e.g. electron and spin density, dipole moments, electrostatic potential. These use semi-empirical methods, e.g. CNINDO, MOPAC or *ab initio* methods, e.g. Gaussian80.
- CHEMGUIDE — a front-end to guide the novice through the command structure, with help and keyword suggestions. This may be useful if the reference manual is not available, but is not recommended for normal use.

### How to use CHEM-X:

- Terminals — You need a graphics screen to get a good display. CHEM-X supports low, medium and high resolution devices. For example, a GIGI (Regis graphics) is low resolution. Only the high resolution devices support the real time interactive functions, e.g. solid fill, bond rotation, zoom.
- Edit your login.com file to include the line @DSKB:[CHEMX]CHEMX.COM to set yourself up for CHEM-X. Then type **CHEMX** to start. The prompt inside CHEM-X is the '\*'. There are worked examples which are best run through step by step. These are a good demonstration for the new user. See page 258 of the manual, and follow the instructions.

There are also files containing structures of some common organic molecules in DSKB:[CHEMX]MOLS.DIR. Use the CHEM-X **READ** command to input any of these structures.

- The manual is available for perusal at the HELP DESK, PCC. It will be necessary to read this to get detailed information on the vast range of options open to you. There is also a copy of the manual at the Computing Services Unit, Griffith University.

- The reference manuals are online in DSKB:[CHEMX]MANUAL.DIR.  
PRIMER.MEM – the primer for novices  
REFTEXT.MEM – the reference manual  
REFHELP.MEM – Help text

For more information about using this program, contact

Dr. Ron Quinn  
c/- Chemistry Dept  
University of Queensland (available during Aug, Nov, Dec 1987)

or

contact the Help Desk, PCC.

*Helen Bergen*  
*ext. 3022*

### **2.3 New VAX LPRINT command**

A new command LPRINT is available on the VAX. It allows the user to print files on the IBM 6670 Laser printer. The service is designed to allow access to the fixed width fonts on the 6670 only. Proportional fonts are not accessible due to the lack of suitable justification software on the VAX. Use the VAX HELP facility for full information on how to use the command. Please read the limitations section under the help command before use. Output is available on A4 sheets of plain white paper. Double-sided printing is available. Note that this facility allows the user to obtain near typewriter quality output. The charges for printing are 4 cents per sheet plus 6 cents per side printed as on the IBM with QPRINT.

*Greg Lehmann*  
*ext. 3022*

## **3. Distributed Computing – Tony Bird, ext. 3391**

### **3.1 Extension of the PC Hire Service**

The hire service has now purchased three Macintosh personal computers for hire to members of staff.

The “Macs” come with 1MB of RAM and 1 × 800KB internal disk drive all in a fetching, blue carrying bag. A basic range of software is also available.

Hiring on of these “Macs” costs the same as the IBM XT Turbos, i.e. \$14.50 per day.

For future details phone the PC Support Group on extension 4233.

*Tony Bird*  
*ext. 3391*

### **3.2 MacEqn – A “Macintosh” Equation Processor**

MacEqn is a desk accessory that provides an environment for writing technical equations for inclusion into documents written with Macintosh word processing programs. MacEqn understands the format of technical equations and provides the user with the ability to include such constructs as integrals, summations, products, superscripts, subscripts, etc. into documents without requiring programs such as MacPaint and MacDraw to create them. An equation can be created while the word processor is active and transferred into the document using the clipboard without leaving the word processor. The equation is drawn in the MacEqn window exactly the way it will appear in print. MacEqn is a large desk accessory, 23K bytes, and requires a 512K Macintosh or larger.

Some examples of MacEqn-formed equations are:

$$E(f_x) = \int_{-\infty}^{\infty} \left[ 1 + \sum_{n=0}^{\infty} \frac{x^n}{n!} \right] \sqrt[3]{1+x^2} e^{-i2\pi f_x x} dx .$$
$$1 + \left[ \frac{1 + \frac{1}{1-x}}{1 + \frac{1}{1+x}} \right]$$

The PC Support Group holds a licence for a copy of MacEqn. For a demonstration or enquiries, phone Chris Barker on ext. 4233.

Tony Bird  
ext. 3391

## 4. Engineering and Communications Services – Graham Rees, ext. 3288

### 4.1 Micom Upgrades – Apology

The upgrade of the MICOM circuit switch as detailed in the next article seemed to cause a great deal of trauma among our users. The major change affecting users was the inability to select a host by number; a symbolic name must now be specified. Unfortunately our pre-upgrade publicity clearly did not reach all clients and for that I apologize.

There are a number of technical reasons for the upgrade concerning increased bandwidth, number of channels and simultaneous calls as well as configuration and diagnostic facilities. These features are not immediately apparent to users – some that are and may be of interest are:

- Improved help facilities. We will be building up this facility in the near future.
- Resource Messages to provide explanations about why hosts cannot be accessed. Again we will be using this feature in the near future.
- Maximum channel speed increased from 9600 bps to 19,200 bps. But don't rush out and set your terminal to 19,200 bps – this speed will operate only on new lines. It may interest some users for special purposes. Any new connections to hosts will be at this speed.
- Forwarding messages on call-setup or clear-downs. This feature is particularly useful for those clients with host connections that do not have modem controls to clear down calls correctly.
- Password protection may be of interest to clients having problems with 'hackers'.

Please contact Graham Jerrard or myself for additional information.

Graham Rees  
ext. 3288

### 4.2 UQ PCC Micom Upgrade

During the weekend of the 11th & 12th of July 1987, the MICOM 600 Circuit Switch of the Prentice Computer Centre was upgraded to a MICOM INSTANET 6600. The INSTANET 6600 has many more features, but the upgrade was not a simple one, involving major changes in both hardware and software. It would be desirable for users to be aware of some of these changes.

Most users are connected to the MICOM circuit switch via variable speed lines. Basically there are two groups, the first accommodating speeds up to and including 2400 baud and the second, speeds up to 9600 baud. Typically users set the desired speed on their terminal and then attempt to communicate with the MICOM. The MICOM must first determine at what speed the user is transmitting and it can only do this, if the user sends a known character first. This character is a CARRIAGE RETURN <CR> (or <ENTER> on some terminals.)

### **Initial Response**

1. Once the MICOM has detected your input and determined the speed it will respond with a welcome message

**Welcome to the UQNET MICOM Circuit Switch.  
Channel ss/ccc SELECT HOST**

2. Then enter the symbolic name of the host computer or facility to which you want to be connected, followed by a <CR>.

**Please Note:** this symbolic name **must** be the **NAME** of that resource in full. Previously the MICOM would accept input here of either a host number or its symbolic name or a unique abbreviation of that name. Now there is no option. A list of the currently available hosts and their symbolic names is given at the end of this article.

3. The MICOM then determines if that user is authorized to be connected to that host and if so completes the connection and outputs to your terminal connected to ss/ccc.

*Note:* In both 1 and 3 above the ss/ccc numbers shown are of the form where ss is a shelf number and ccc is a channel number and thus the user is now informed of the incoming channel via which the connection is being made and the outgoing channel through which the host computer will be addressed. These numbers would be helpful for fault reporting in the event of trouble.

4. The user is now connected to the host computer or other facility. This host must now determine the speed of the terminal and MICOM connection so enter another <CR> or two until the host responds.

The connection through the MICOM is now transparent apart from the <BREAK> character which is used to signal the MICOM that the user wishes the MICOM to break or disconnect that connection.

### **Breaking a Connection**

At the end of a session the user would normally log off the host computer which in most cases automatically breaks the connection through the MICOM, and results in the **SELECT HOST** message being received again with the opportunity to select a different host. If no host name is entered within 12 seconds, the MICOM will send a **DISCONNECTED** message and break the connection. If the user wishes to physically break the connection through the MICOM for some reason, the <BREAK> key on the terminal is used. Another change has been included here, in that for most users now, 3 short breaks in fairly quick succession must be entered. This has been done to guard against accidental use of the <BREAK> key.

If the <BREAK> key sequence is used while logged on to a computer host, the MICOM will break the connection and send a **DISCONNECTED** message to the user, but the action then taken by the computer system varies, depending on the computer operating system. This practice is not encouraged. If possible, log off the computer system before entering the break sequence.

### **Other Features**

#### **Direct Addressing**

Users lines may be enabled to allow direct addressing of a given computer port or another users line. This may have application for PC users wishing to transfer files between users as an example. To use this feature it is first necessary to know the channel to which the other user is connected. Using a user who is connected to

channel 5/103 as an example, access the MICOM as usual to the point where the welcome message and the **CHANNEL ss/ccc SELECT HOST** message is received, then instead of entering the symbolic name of the desired host, enter **#5/103<CR>** and the connection to that users line will be completed.

### Fixed Destination/Default Destinations

Individual users lines or groups of lines (e.g. within a terminal laboratory) may be restricted to a fixed destination where users do not receive the **SELECT HOST** message but are automatically connected to a pre nominated channel or host.

The users line may also be configured with a default channel or host so that after receiving the **SELECT HOST** message, a **<CR>** will automatically connect to that pre-defined channel or host. This may be useful for users who invariably use the one host, but on some occasions need to be able to nominate other hosts.

### Password Protection

The MICOM now allows for two levels of password protection. An incoming users channel may be configured so that a pre-defined password must be correctly entered before the MICOM will allow access to the resources controlled by it.

A second level of password protection may be used either in addition to the first or by itself, such that after the user enters the HOST name, the MICOM will insist that a password applying to that host only, must be correctly entered before connecting a potential user. This resource password may be of use to departments who have their departmental computer ports connected to the PCC MICOM, and whose intended users can all be advised of the current password which would be entered and updated in the MICOM on advice from the department controlling the resource. This feature may be helpful in protecting departmental resources whose own operating systems do not have adequate access protection from unauthorized users.

The MICOM passwords must be set and controlled by the Prentice Computer Centre. Users interested in this level of security should contact Graham Rees or myself for further details.

### General

Other new features are also available but probably are not of general interest. Any user who has a specific need or application, should call Graham Jerrard on 377 3168.

### HOSTS

SYMBOLIC NAME	COMPUTER or FACILITY	SYMBOLIC NAME	COMPUTER or FACILITY
AUSPAC	X-25 PAD TO AUSPAC	KEMENG2	CHEMICAL ENGINEERING PDP 11/03
CADCAM	COMPUTER-VISION CAD-CAM	MATHP	MATHEMATICS – PYRAMID – UNIX
CLAYTONS	TWO CROSS CONNECTED CHANNELS	MATHS	MATHEMATICS – ZILOG – UNIX
COMPSCI	COMP. SCIENCE UNIX FOR STUDENTS	PHILOS	PHILOSOPHY – ALTOS
EXSTUD	EXTERNAL STUDIES VAX 11/750	PSYCH	PSYCHOLOGY
GRIFIN	GRIFFITH UNI PDP 11/34	UNIX	COMP. SCIENCE PERKIN ELMER 3200
GUCIS	GRIFFITH UNI VAX 11/750-ULTRIX	UQADM	VAX 8650 ALL USERS
GUBEAM	GRIFFITH UNI SCIENCE LASER LAB PDP 11/23	UQKL10	KL10 FOR GENERAL USE
GUDATA	GRIFFITH UNI PDP 11/23	UQVAX	VAX 11/780 FOR GENERAL USE
GUMVAX	GRIFFITH UNI MICRO-VAX	UQVM	DUMMY TO ROUTE USERS TO uqvma, uqvmb or uqvmc
GUOLIVE	GRIFFITH UNI OLIVETTI	UQVMA	IBM VIA SERIES 1 no 1
KEMENG	CHEMICAL ENGINEERING PDP 11/40	UQVMB	IBM VIA SERIES 1 no 2
		UQVMC	IBM VIA SERIES 1 no 4
		WOMBAT	PCC ENGINEERING MICRO-VAX 2

Graham Jerrard  
ext. 3168



## 5. Applications Development – Sarah Barry, ext. 4281

### 5.1 Information Concerning Courses

Enrolments for all courses may be made by phoning extension 3018.

The following courses will be offered during the period September–December 17, 1987:

#### September

‡Introduction to MS/PCDOS	September 7–9 3 half-days 9–12am each day
‡Introduction to WORDPERPECT Typesetting (on KL–10)	September 7–10 4 half-days 1–4pm each day
†Introduction to DATATRIEVE	September 7–11 5 half-days 9–12am each day
‡“Desk-Top Publishing” Overview	September 14–18 5 half-days 9–12am each day
•Introduction to SQL	September 16 1 half-day 1–4pm
‡Introduction to WORDPERFECT	September 21–25 5 half-days 9–12am each day
•Text Facilities on IBM3083E	September 21–24 4 half-days 1–4pm each day
‡Introduction to DBASE III	September 23–24 2 half-days 1–4pm each day
•Introduction to IBM3083E	September 29–October 1 3 half-days 9–12am each day
	September 29–October 2 4 half-days 9–12am each day

#### October

‡Introduction to WORDPERFECT	October 5–8 4 half-days 1–4pm each day
‡Introduction to MS/PCDOS	October 7–9 3 half-days 9–12am each day
‡“Desk-Top Publishing” Overview	October 14 1 half-day 9–12am
†•General Plotting	October 20–23 4 half-days 9–12am each day
‡Introduction to DBASE III	October 21–23 3 half-days 9–12am each day
†RUNOFF	October 26–30 5 half-days 1–4pm each day

## November

•Introduction to IBM3083E	November 2-5 4 half-days 1-4pm each day
‡Introduction to WORDPERFECT	November 2-5 4 half-days 1-4pm each day
‡Introduction to MS/PCDOS	November 3-5 3 half-days 9-12am each day
•Introduction to SQL	November 9-13 5 half-days 1-4pm each day
‡Introduction to DBASE III	November 10-12 3 half-days 9-12am each day
‡PC-to-Mainframe Communications	November 16 1 half-day 9-12am
†Introduction to VAX	November 17-19 3 half-days 9-12am each day
‡PC Overview	November 18 1 half-day 9-12am
†•Introduction to SPSS-X	November 23-27 5 half-days 1-4pm each day
‡“Desk-Top Publishing” Overview	November 25 1 half-day 9-12am
‡Introduction to Programming in BASIC	November 30-December 4 5 half-days 9-12am each day
•Introduction to SAS	November 30-December 4 5 half-days 1-4pm each day
‡Introduction to WORDPERFECT	November 30-December 3 4 half-days 1-4pm each day

## December

Typesetting (on KL-10)	December 7-11 5 half-days 9-12am each day
‡Introduction to MS/PCDOS	December 8-10 3 half-days 9-12am each day
†•Introduction to Programming in FORTRAN	December 14-18 5 full days 9-12am + 1-4pm each day
‡Introduction to DBASE III	December 15-17 3 half-days 9-12am each day

• denotes IBM course

† denotes VAX course

If marked † please indicate when enrolling whether you would prefer your course account to be established on the VAX or IBM machine.

‡ denotes PC course

*General Notes:*

1. It is expected that users attending courses on specific packages (SQL, SAS, SPSS-X, DBASE III, etc) will be familiar with terminal-usage, file-management and editing on the relevant machine (IBM, VAX or PC). Attendance at such short courses without this background provides many problems, as all courses are hands-on. Introductory courses are given frequently to allow familiarity with the fundamentals *before* attending courses on particular application packages.
2. All courses will be held in the Centre's teaching rooms near the Physics Annexe – the mainframe courses in Course Room 1 and the micro-computer courses in Course Room 2.
3. Staff, post-graduate students and kit-owners are admitted free to courses. The charge is \$10.00 per half-day session for other internal users; \$17.00 per half-day session for affiliated users; and \$37.00 per half-day session for external users.
4. Enrolments for all courses may be made by phoning ext. 3018.

*Barry Maher/Nick Evans  
ext. 3021*

