COMPUTING ENVIRONMENT AT C-MMACS

High Performance Computing

Major enhancement of facilities took place during the reporting year. CONVEX C3820 supercomputer was thrown open to user groups in April 94, and it was put on round-the-clock operation. Its utilisation, which exceeded 9000 CPU hours during 1994-95, shows that it is extremely popular amongst scientists of several disciplines (Figs. 17 and 18). Four high performance graphics workstations (two INDIGO 2, and two ALPHAs 3000/800) were installed and commissioned in September 1994. They have been extensively used for pre- and post-processing tasks, especially for three-dimensional problems.

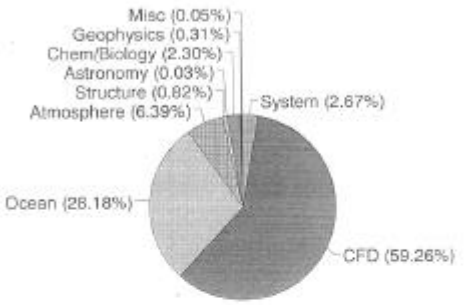

Figure 17: Discipline wise break-up of utilisation of the CONVEX supercomputer at C-MMACS during 1994-95

Networking

The local area network (LAN) for C-MMACS, built around an UNGERMANN BASS bridge/router and an FDDI ring, was installed, tested and put in operation in August 1994. The network has proved to be extremely useful and reliable. (See inside back cover.) The wide area network (WAN) connectivity was strengthened by sustained efforts to improve the uptime and throughput of the leased line connecting C-MMACS and the ERNET node in IISc. INTERNET operations, which began in March 1994, were improved and a class C address (202.41.64.0) was given to C-MMACS network in October 1994. These facilities have been extensively used for transferring large data files, public domain software and for other communications. Also, it was demonstrated that C-MMACS computing resources, including CONVEX C3820, can be used remotely through INTERNET as well as dial-up connections. Industries in Bangalore have begun using this facility.

Software

Several software packages were procured and installed on CONVEX (e.g., TIDAL, PORFLOW, AMBER, XPLOR, BERNESE etc.) Table II gives major software packages.

E-mail Services

C-MMACS continued to offer e-mail services to a large number of users in C-MMACS and

NAL. The number of users was over 100 on March 31, 1995. Typically over 80 incoming and outgoing messages were handled everyday and the volume of information transmitted was over 500 KB /day.

Consultancy and Other Services

C-MMACS provided technical advice to National Institute of Oceanography(NIO), Goa on setting up a campus wide local area network. C-MMACS also provided consultancy services to the Delhi University on benchmarking of compute-server, file-servers and workstations. C-MMACS is presently engaged in assisting CSIR HQ in selecting computer systems for IMPACT and other applications. Furthermore, training was provided to 30 students and graduates. Also, research students of the Bangalore University and the J.N. University availed of C-MMACS computing facilities and expertise.

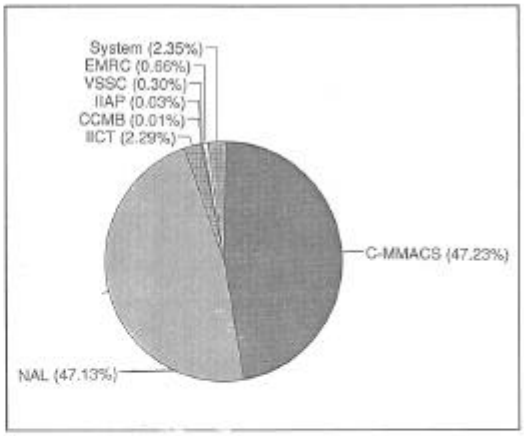

Figure 18: Break-up of utilisation of CONVEX supercomputer at C-MMACS during 1994-95 according to institutions

(R P Thangavelu, A Saldanha, K S Yajnik, H Krishnamurthy, * IISc)*

Table II

The Software at C-MMACS

Mathematical Libraries

DXML	Extended Mathematical Libraries	ALPHA
EISPACK	Eigen System Analysis	COSMOS
ELLPACK	Solvers for Elliptic Partial Differential Equations	CONVEX
IMSL	Comprehensive Library for Numerical and Statistical Analysis	INDIGO2, COSMOS, PS/386
ITPACK	Iterative Solvers for Linear Systems	COSMOS, CONVEX
LAPACK	Linear Algebra	CONVEX
LINPACK	Linear System Solvers	COSMOS, CONVEX
NAG	Numerical & Statistical Analysis	PS/486
NUMERICAL RECIPES	Extensive Programmes of Numerical and Statistical Analysis	COSMOS, PS/386 CONVEX
ODEPACK	Ordinary Differential Equation Solvers	COSMOS, CONVEX
SPARSEPACK	Sparse Linear System Solvers	COSMOS, CONVEX
VECLIB	CONVEX vector libraries	CONVEX

Application Packages

Biology & Chemistry

AMBER 4	Modelling of Peptides/Nucleic Acids/Carbohydrates	CONVEX,COSMOS, SUN
CHEMKIN	Chemical Kinetics	COSMOS, CONVEX
GROMOS	Modelling of Peptides/Nucleic Acids/Carbohydrates	CONVEX, COSMOS
NASACEC	Chemical Equilibrium (Combustion)	COSMOS, CONVEX
MOPAC 6	Molecular Orbital Calculations	CONVEX, COSMOS
PCMODEL	Molecular Modelling	IRIS
XPLOR	X-ray crystallographic and solution NMR structure determination	CONVEX

CAD/CAE

AUTOCAD	Computer Aided Design	PS/386
CAMAND	Computer Aided Modelling, Analysis Numerical Control, Design and Documentation	IRIS
SDRC I-DEAS	Solids Modelling	IRIS

Scientific Visualisation

AVS	Application Visualisation System	CONVEX
GrADS	Graphical display for atmospheric and oceanic apllications	INDIGO2, ALPHA
NCAR Graphics	Advanced graphics display with mapping capabilities	INDIGO2, SUN, IRIS
CHITRA	Graphics for CFD	INDIGO 2

Structural Mechanics

NISA	Finite Element Analysis	CONVEX, PS/486
SDRC I-DEAS	Finite Element Modelling	IRIS

Miscellaneous

ACRPLOT	General Purpose Plotting Package	PS/486
CSS STATISTICA	Integrated Statistical and Graphics analysis	PS/386
DADISP	Digital Signal Processing	PS/386
DT-IRIS	Image Processing Software	PS/386
MAPINFO	Desktop Mapping Sotware	PS/386
MATLAB	High Performance Matrix Computation	PS/386
NEXPERT	Expert System Shell	PS/386

Graphics Libraries

GINO-F	PS/386
GINOGRAF	PS/386
GINOSURF	PS/386
GKS	INDIGO2, COSMOS
GL	INDIGO2, IRIS
NAG Graphics	PS/486
OpenGL	INDIGO2, ALPHA
PHIGS	INDIGO2, ALPHA, SUN
X11R5	CONVEX, INDIGO2, ALPHA