COMPUTING ENVIRONMENT

High Performance Computing

The high performance computing and networking resources of the centre with a robust Internet link, which are operational round-the-clock, continue to grow and provide efficient service to the scientists of C-MMACS, NAL and other CSIR laboratories. The uptime efficiency of the computing environment was maintained at above 98% during the year 1996-97. The Convex C3820 supercomputer recorded an utilisation of 12,246 CPU hours during the year 1996-97 and the total utilisation since its installation has crossed 35,000 CPU hours. The system has been used extensively for various programmes of ocean modelling. Additional memory has been installed on DEC Alpha and SGI Indigo-2 workstations to improve the computing capabilities of these systems. The computing resources have been further augmented by adding two numbers of Ultra Sparc workstations.

Network and Hardware Enhancement

The Local Area Network (LAN) has been extended to the entire first floor of C-MMACS building and the expanded network became operational in May 1996. 3com hubs have been added to provide network connection to more systems in various segments of the LAN. Six numbers of SGI Indy workstations were installed and commissioned on the LAN. These machines configured with NIS and NFS are used as front-end systems to Convex C3820 and other high performance workstations. A PC network, consisting of a Compaq pentium server with Banyan Vines network operating system and 20 pentium desktop machines, has been integrated into the existing TCP/IP based ethernet LAN. With this addition, the computing resources are accessible from the desktop of every individual scientist at C-MMACS. Network print services were improved by adding a Tektronix Phaser 340P colour postscript printer, a HP Laserjet 4Mplus printer and a Lantronix EPS-2 multiprotocol printserver on the LAN.

Internet Services

Internet connectivity has been strengthened by adding a CISCO 2522 router for the WAN link. An SGI WebFORCE Indy web server has been installed, configured and commissioned in November 1996. The URL for the home page of C-MMACS is http://www.cmmacs.ernet.in. An anonymous FTP server was configured and set-up, and can be accessed at the address ftp.cmmacs.ernet.in.

The Centre continues to provide Internet services (www, ftp, e-mail etc.) to a large number of users from C-MMACS and NAL. There were over 200 registered users as on March 1997. Web server facilities are provided to over 75 users of C-MMACS and NAL. E-mail subnode facility has been extended to Flosolver unit at NAL Kodihalli campus.

Software

Upgrades and new versions of operating systems and several application software packages have been installed on the high performance computing platforms. In addition a network license for MATLAB across platforms, workstation versions of SPSS and Framemaker were procured and installed. The following list gives the software packages available, along with a brief description and the platforms on which they are ported.

Biology & Chemistry

AMBER 4	Modelling of peptides / nucleic acids / carbohydrates	CONVEX, COSMOS, SUN
GROMOS 95	Modelling of peptides / nucleic acids / carbohydrates	CONVEX
MOPAC 6	Molecular orbital calculations	CONVEX, COSMOS
PCMODEL	Molecular modelling	SGI
XPLOR	X-ray crystallographic and solution NMR structure determination	CONVEX

CAD/CAE

CAMAND	Computer aided modelling, analysis, numerical control, design and documentation	SGI
CFD-GEOM	Surface modelling and grid generation	SGI
SDRC I-DEAS	Solid modelling	SGI

Earth Sciences

BERNESE	GPS data processing	SUN
CCM 2	Community climate model	CONVEX
FASCOD 2	Line-by-line atmospheric radiative transfer	COSMOS
LOWTRAN 7	Atmospheric radiative transfer	CONVEX, COSMOS
MOM	Global ocean circular (Modular model)	CONVEX, DEC, SUN
TIDAL	Shallow water simulation and pollutant transport	CONVEX, INTEL

Fluid Flow, Heat and Mass Transfer

CFD-ACE	Computational fluid dynamics	CONVEX
NISA	Finite element fluid dynamics code	CONVEX, INTEL
PHONENICS	Computational fluid dynamics	CONVEX, INTEL
PORFLOW	Porous media flow, heat and mass transfer	CONVEX, INTEL

Graphics Libraries

GKS		SGI, COSMOS
NAG Graphics		CONVEX, INTEL
PHIGS		SGI, DEC, SUN

Mathematical Libraries

DXML	Extended mathematical libraries	DEC
EISPACK	Eigen-system analysis	COSMOS
ELLPACK	Solvers for elliptic partial differential equations	CONVEX
IMSL	Comprehensive library for numerical and statistical analysis	SGI , COSMOS, INTEL
ITPACK	Iterative solvers for linear systems	CONVEX, COSMOS
LAPACK	Linear algebra	CONVEX
LINPACK	Linear system solver	CONVEX, COSMOS

NAG	Numerical and statistical analysis	CONVEX, SGI, INTEL
ODEPACK	Ordinary differential equation solvers	CONVEX, COSMOS
SPARSEPACK	Sparse linear system solvers	CONVEX, COSMOS
VECLIB	CONVEX vector libraries	CONVEX

Scientific Visualisation

AVS	Application visualisation system	CONVEX
CFD-VIEW	Graphics for CFD	SGI
GrADS	Graphical display for atmospheric and oceanic applications	SGI, DEC
NCAR Graphics	Advanced graphics display and mapping	SGI, SUN
TECPLOT	General purpose 3-D graphics	SGI, INTEL

Structural Mechanics

NISA	Finite element analysis	CONVEX, INTEL
SDRC I-DEAS	Finite element modelling	SGI

Miscellaneous

ACRPLOT	General purpose plotting package	INTEL
STATISTICA	Integrated statistical and graphics analysis	INTEL
MATLAB	Mathematical and symbolic computation	DEC, INTEL
NEXPERT	Expert system shell	INTEL
SPSS	Advanced statistical analysis	DEC

Other Services

Technical advice has been provided to NAL, Bangalore and CFRI, Dhanbad towards setting up a campus wide local area network. Computing resources have also been provided to research students of Bangalore University. In addition, students from Birla Institute of Technology and Science, Cochin University of Science and Technology, Madurai Kamaraj University and University of Mysore have also availed the computing facilities.

Ongoing Enhancement

Following are the systems under procurement to augment the computing resources of C-MMACS.

1. Three numbers of R10000 CPU based SGI O2 workstations.
2. One number of R10000 based SGI Origin 200 server with 4 CPUs.
3. Memory upgradation of Indy work-stations.

In addition, an optical fibre communication link between C-MMACS and NAL Belur campus is being set-up with technical help from C-MMACS.
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