

## 5. COMPUTING ENVIRONMENT

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### High Performance Computing

The SGI Origin 200 server (O200) continues to be the mainstay of the computing environment, after Convex C3820 was retired in February 2000, and has catered to the computing needs of the users to the best of its ability. The server was made available to users on a round-the-clock basis with almost 100% uptime efficiency. The total usage of O200 during the year 2000-01 stood at 17,797 CPU hours. Of this, about 39% was utilised by scientists from C-MMACS while the remaining 61% was utilised by scientists from NAL and other CSIR laboratories as well as a few other academic institutions.

The compute performance of the O200 improved after the commissioning of the IBM SSA based, high-availability NFS server which shifted NFS load from O200 to the IBM NFS server. An additional 2 GB memory has been added to the O200 server to meet the growing needs. Further, purchase order has been placed for the upgradation of the 4x180 MHz MIPS R10000 processors to 4x360 MHz MIPS R12000 processors which is expected to double the performance of the server. Nevertheless, it was quite clear that the computing needs at C-MMACS far outweighs what O200 can deliver.

A thorough study of the features and architectures of major compute servers available in the market, including the indigenously built parallel computers, was carried out to identify the potential candidates to meet the growing computing requirements at the Centre; the INDOMOD project was prepared to fund the computer server. A tender was released for the procurement of a Large Compute Server (LCS) with detailed specifications as approved by the Technical Evaluation Committee (TEC). The tender also included a performance evaluation through benchmarking of various servers using a benchmark test based on a one month sample run of the Modular Ocean Model, version 3 (MOM3). One of the major criteria to decide on the required configuration was the ability to run the benchmark model within 40 minutes, while also requiring that this configuration should be easily upgradable to one that can run the model

within 20 minutes. The technical and performance evaluation of the proposals submitted by various vendors is being carried out\*.

### Hardware addition

A SGI Octane2 workstation, with dual R12000 processors, 512 MB main memory, V6 graphics accelerator and 18 GB disk capacity, has been added to the computing environment recently in addition to a couple of SGI O2 workstations and a few Intel Pentium III desktop systems; the Octane2 workstation is meant for running CAMAND and I-DEAS software. One of the Pentium III systems is configured as a Linux server and a number of public domain softwares will be made available on this server to help scientists in carrying out computing jobs which require moderate computing power.

### EPABX remote shelf at C-MMACS

In order to improve the voice communication facility at C-MMACS, a remote shelf for the new telephone exchange at the NAL Belur Campus was installed and commissioned at C-MMACS, using the existing single mode fiber cable. Direct dialing to individual extensions (DID) will become possible with the DID facility expected to be available in the near future.

### E-mail and Internet Facilities

E-mail services are being provided to more than 700 users through C-MMACS mail gateway. C-MMACS staff members were provided with an alternate connectivity to Internet through the 512 kbps link from NAL Kodihalli campus. C-MMACS web pages are being regularly updated and news clips of important events related to C-MMACS are being maintained; information about C-MMACS activities related to Bhuj earthquake is hosted on the C-MMACS web site.

A Simple Network Management Protocol (SNMP) based bandwidth monitoring package for the Internet access link has been developed, which gives the actual

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\*At the time of going to the press, the procedures are finished and an order has been placed for the supply of SGI Origin 3400 server with 16x500 MHz MIPS R14000 processors, 16 GB main memory, 140 GB of RAID storage and Gigabit network interfaces. The new server is likely to be installed in August 2001. TEC had shortlisted Compaq GS160/320 & SGI Origin 3400 servers. Based on the price and performance, purchase order was placed for the above. Upon installation, this server will be one of the most powerful computer systems in the country.

utilization of the 64 kbps link to ERNET through STP. This is expected to help in deciding about the required enhancement of infrastructure and network security as and when required.

## Softwares

CFD-ACE+ has been upgraded to version 6. Public domain softwares like Netcdf, Gnu plot and Grads were upgraded

to their respective new versions. General Circulation Model (GCM) from LMD, France is being ported from Solaris to IRIX platform. The Generic Mapping Tools (GMT) software and SCILAB software for mathematical and symbolic computation were also installed on the O200. A table is provided below listing the available softwares at C-MMACS, in various categories, with the name, description and platform(s) on which they are available given in the first, second and third columns, respectively.

### Mathematical Libraries

Complib	High performance math libraries	SGI
DXML	Extended mathematical libraries	DEC
IMSL	Comprehensive library for numerical and statistical analysis	SGI, Intel
NUMERICAL RECIPES	Software for numerical analysis	SGI, Intel
SCSL	SGI Cray scientific library	SGI

### Application Packages

#### *Biology & Chemistry*

AMBER	Modelling of peptides / nucleic acids / carbohydrates	SGI, SUN
DeFT	Gaussian density functional program	SGI
deMon-KS	Molecular orbital solution of the Kohn-Sham DFT system of equations	SGI
PCMODEL	Molecular modelling	SGI

#### *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	SGI, SUN
MOM	Global ocean circulation (Modular model)	SGI, DEC, SUN
TIDAL	Shallow water simulation and pollutant transport	SGI, Intel

#### *Fluid Flow, Heat and Mass Transfer*

CFD-ACE+	Computational fluid dynamics	SGI
NISA	Finite element fluid dynamics	SGI
PHONENICS	Computational fluid dynamics	SGI
PORFLOW	Porous media flow, heat and mass transfer	Intel

#### *Scientific Visualisation*

CFD-VIEW	Graphics for CFD	SGI
Ferret	Visualisation tool for atmospheric and oceanic applications	SGI
GrADS	Graphical display for atmospheric and oceanic applications	SGI, DEC

NCAR Graphics	Advanced graphics display and mapping	SGI, SUN
SigmaPlot	Data manipulation, regression and curve fitting	Intel
SigmaScan Pro	Image digitising software	Intel
TableCurve 2D	Automated curve fitting and equation discovery	Intel
TableCurve 3D	Automated surface fitting and equation discovery	Intel
TECPLOT	General purpose 3-D graphics	SGI, Intel

### **Structural Mechanics**

NISA	Finite element analysis	SGI, Intel
SDRC I-DEAS	Finite element modelling	SGI

### **Miscellaneous**

ACRPLOT	General purpose plotting package	Intel
AXUM	Technical Graphics and Data Analysis	Intel
CSS STATISTICA	Integrated statistical and graphics analysis	Intel
FLOWPATH	2-D flow and contaminant transport in sub-surface	Intel
GMT	Generic Mapping Tools	SGI
GNUPLOT	General purpose plotting package	SGI
MACSYMA	Applied Mathematics software	SUN, Intel
MATLAB	Mathematical and symbolic computation	SGI, Intel
MathCAD	Mathematical calculation, visualisation and documentation	Intel
MODFLOW	3-D simulation of flow in sub-surface	Intel
NEXPERT	Expert system shell	Intel
PdEase	Applied Mathematics software	SUN, Intel
SCILAB	Mathematical and symbolic computation	SGI, Intel
SPSS	Advanced statistical analysis	DEC
Trivoli ADSM	Automatic backup management software	IBM
Visual MODFLOW	3-D flow and contaminant transport in sub-surface	Intel

### **Graphics Libraries**

GKS	Graphical Kernel System	SGI
NAG Graphics	Graphics Libraries	SGI
PHIGS	Graphics Libraries	SGI, DEC

### **Other Services**

Technical advice has been provided to CMRI, Dhanbad in setting up of a switch based Local Area Network (LAN) connecting various buildings at different locations of the campus. Technical advice was provided to IICT, Hyderabad for improving the LAN setup and also to enhance the Internet bandwidth. Operation, maintenance and data archival of GPS station at IISc were carried out from October 2000 to January 2001. Consultancy services were provided to Centre for Air Borne Systems, Bangalore for the design, implementation and operation of their campus wide LAN and MIS. Consultancy services were also provided to the

All India Institute for Speech and Hearing, Mysore for the design and implementation of a campus LAN. Optimisation and debugging of a computational material science code from RRL, Trivandrum was carried out and computing services were provided to them using this code. Computing facilities were provided to Ph.D. students from IIT, Delhi and Bangalore University for carrying out their research work. In addition, computing resources were provided to the students of various universities enabling them to carry out their academic project works.

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