

5. COMPUTING ENVIRONMENT

High Performance Computing

The SGI Origin 200 server with four processors has remained as the major file-cum-compute server during the year 1999-2000. The Origin 200 server has been extensively utilised by the scientists of C-MMACS, NAL and other CSIR laboratories to meet their computational requirements in modelling and simulation. The server was available to users on the network on a round-the-clock basis with almost 100% uptime efficiency.

In February 2000, the Convex C3820 supercomputer was retired, after providing six years of excellent computing service, due to lack of availability of technical support and spare parts from HP-Convex and non- Y2K-compliant hardware and software.

Procurement and installation of an IBM, serial storage architecture (SSA) based, highly available Network File system (NFS) server, in the later part of the year, has taken over the NFS load from Origin200. This file server consists of, (a) two numbers of identically configured IBM RS/6000 model H70 servers, (b) an IBM SSA 7133 storage subsystem configured with 576GB (16 x 36GB) of hard disk capacity in a RAID 5 environment and, (c) two numbers of Digital Linear Tape (DLT) library subsystems. Each of the H70 servers is configured with two numbers of RS64-II processors running at 340 MHz and with 512 MB main memory. The servers are clustered using Highly Available NFS (HANFS) cluster software for high availability with failsafe mechanism.

The process of procuring a large compute server, to replace the Convex C3820 and to meet the growing computational demands of large scale models, has been initiated with the constitution of a high level committee. A preliminary survey of available computing platforms has been made to facilitate the procurement process. Also, benchmark procedures have been drawn up, using a large scale ocean model, to evaluate the performance of compute servers so as to enable the committee to decide on a suitable system.

Year 2000 Compliance

The Y2K rollover at C-MMACS was smooth and there were

no serious problems. An internal committee constituted by Scientist-in-Charge, C-MMACS carefully examined the status of Y2K readiness of the High Performance Computing Centre and took necessary steps to make the same Y2K ready. Though the Convex C3820 and DEC Alpha systems could not be tested for Y2K readiness, the rollover was smooth. All SGI workstations and servers were made Y2K ready by applying the required patches for the operating system and compilers, while the operating systems of the Sparc workstations were upgraded to Solaris 7 to make them Y2K ready. The Compaq Prosignia 500 servers were made Y2K ready by upgrading the firmwares of the system and by applying patches for SCO Unix operating systems. The Pentium and Pentium II systems were made Y2K ready by upgrading the BIOS and by applying required patches. The general purpose and scientific software, which were not Y2K ready, were upgraded to their respective Y2K compliant versions.

Campus Networking

A gigabit inter-campus backbone network has been installed and commissioned between the campuses of C-MMACS, NAL-Kodihalli, and NAL-Belur. This network provides a redundant path between the different campuses, in a triangular connection, using sophisticated multi-layer Ethernet routing switches (Cabletron SSR 2000) over single mode optical fibre cable. The campus network is sub-netted into multiple IP networks using class C private IP address scheme. This has enabled the scientists in both the campuses of NAL to access C-MMACS facilities through the network.

Software

Tivoli ADSM software has been installed on the newly commissioned IBM file server for backup management using the DLT tape libraries. Bernese software, for GPS data processing, was upgraded to version 4.2. CFD-ACE+ has been upgraded to version 5.4 and NISA was upgraded to version 9. A table is provided here listing the existing softwares at C-MMACS, in the various categories, with *the name, description and the 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
NAG	Numerical and statistical analysis	SGI
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
PHOENICS	Computational fluid dynamics	SGI
PORFLOW	Porous media flow, heat and mass transfer	Intel

Scientific Visualisation

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
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

ACRLOT	General purpose plotting package	Intel
AXUM	Technical Graphics and Data Analysis	Intel
CSS STATISTICA	Integrated statistical and graphical analysis	Intel
FLOWPATH	2-D flow and contaminant transport in sub-surface	Intel
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
SPSS	Advanced statistical analysis	DEC
Tivoli ADSM	Automatic backup management software	IBM RS/6000
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 NAL in the setting up and operation of the optical fibre based gigabit inter-campus backbone network. Consultancy services were provided to Centre for AirBorne Systems for the design, implementation and operation of the campus wide LAN. Computing resources were provided to the students of Bangalore University, Cochin University of Science and Technology, Madurai Kamaraj University, Mangalore University, Bharathidasan University and University of Madras enabling them to carry out their academic project works.

In order to increase the visibility of NAL and C-MMACS

pages on the web, we came up with an interesting idea of organising a World Cup Cricket contest. Gobind Patra of IMD, NAL implemented a professional contest on the web using CGI and Java scripts and PERL. Dr. Srinivas Bhogle, Head, IMD provided prizes for the contestants. In spite of the short time the contest stayed open (it was open for only a week), we received 800 entries from all parts of the world, possibly the largest number of hits C-MMACS received in a single week of its history.

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