5. COMPUTING ENVIRONMENT

High Performance Computing

The Convex C3820 computer system has successfully completed five years of excellent computing service to the scientists of C-MMACS and other CSIR laboratories. The total utilisation of C3820 has crossed 50,000 CPU hours. The system continues to be maintained in-house with technical advice and spares support from HP-Convex, Singapore.

Upgradation of the 4 CPU Origin 200 server was completed and the system is now configured with 1 GB memory and 72 GB disk storage. The Origin 200 now functions as a file cum compute server and caters to the NFS requirements of users across the LAN with almost 100% uptime efficiency.

Hardware enhancement

Five numbers of IBM Pentium II workstations (64 MB memory, 4 GB disk) were added to the LAN to improve the availability of high end desktops for scientific applications. Three numbers of pentium systems were also added to the network for general purpose use along with a CD-Writer for data archiving.

A single CPU Origin 200 server has been installed and commissioned for improved network services. Two numbers of DLT drives with a capacity of 15 GB (30 GB compressed) each have been added to the LAN for high speed backup across the network.

Internet services

The 64 Kbps VSAT link to CSIR has been commissioned and put into operation for a specified time slot on every day and is expected to be operational on a full time basis once the required transponder space is allotted to CSIR.

A web based live access server has been installed and made operational on the C-MMACS web server for serving the Modular Ocean Model data and other oceanic & climate data to researchers in ocean, atmosphere and climate science.

In order to facilitate the smooth functioning of the JGOFS International Indian Ocean Symposium and training course during January 1999, a computing environment was set

Mathematical Libraries

DXML	Extended mathematical libraries	DEC
ELLPACK	Solvers for elliptic partial differential equations	Convex
IMSL	Comprehensive library for numerical and statistical analysis	SGI , Intel
NUMERICAL RECIPES	Software for numerical analysis	SGI, Intel
ITPACK	Iterative solvers for linear systems	Convex
LAPACK	Linear algebra	Convex
LINPACK	Linear system solver	Convex
NAG	Numerical and statistical analysis	Convex, SGI
ODEPACK	Ordinary differential equation solvers	Convex
SPARSEPACK	Sparse linear system solvers	Convex
VECLIB	Convex vector libraries	Convex

Application Packages

Biology & Chemistry		
AMBER	Modelling of peptides / nucleic acids / carbohydrates	Convex, SUN
DeFT	Gaussian density functional program	SGI, Convex
deMon-KS	MO solution of the Kohn-Sham DFT system of equations	SGI, Convex
GROMOS	Modelling of peptides / nucleic acids / carbohydrates	Convex
MOPAC	Molecular orbital calculations	Convex
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	SGI, SUN
CCM 2	Community climate model	Convex
LOWTRAN 7	Atmospheric radiative transfer	Convex
MOM	Global ocean circulation (Modular model)	SGI, Convex, DEC, SUN
TIDAL	Shallow water simulation and pollutant transport	Convex, Intel
Fluid Flow, Heat and Mass Transfer		
CFD-ACE	Computational fluid dynamics	Convex, SGI
NISA	Finite element fluid dynamics code	Convex, SGI
PHONENICS	Computational fluid dynamics	Convex, SGI
PORFLOW	Porous media flow, heat and mass transfer	Convex, Intel
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
AXUM	Technical graphics and data analysis	Intel
CSS STATISTICA	Integrated statistical and graphics analysis	Intel
MATLAB	Mathematical and symbolic computation	SGI, Intel
MathCAD	Mathematical calculation, visualization and documentation	Intel
NEXPERT	Expert system shell	Intel
SPSS	Advanced statistical analysis	DEC
MACSYMA	Applied Mathematics software	SUN, Intel
PDEase	Applied Mathematics software	SUN, Intel
Graphics Libraries		
GKS		SGI
NAG Graphics		Convex, Intel
PHIGS		SGI, DEC, SUN

up at the symposium venue consisting of workstations and PCs on a LAN with a full fledged internet and mail node. Each participant was given a separate account to provide individual access.

An internet proxy server has been installed at C-MMACS for a faster access to internet and also to enable access control.

Software

New application softwares have been added to the large

pool of existing softwares at C-MMACS and information on the availability of various softwares with the associated platforms is listed in the table below.

Other Services

Computing services were provided to scientists from various CSIR laboratories. Technical advice has been provided to NAL in settig up a gigabit campus network. Students of Bangalore University, Bharathidasan University, Birla Institute of Technology and Science, Cochin University of Science and Technology, Mangalore University and Nagarjuna University were provided computing facilities to carry out their respective academic project works at C-MMACS.

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