

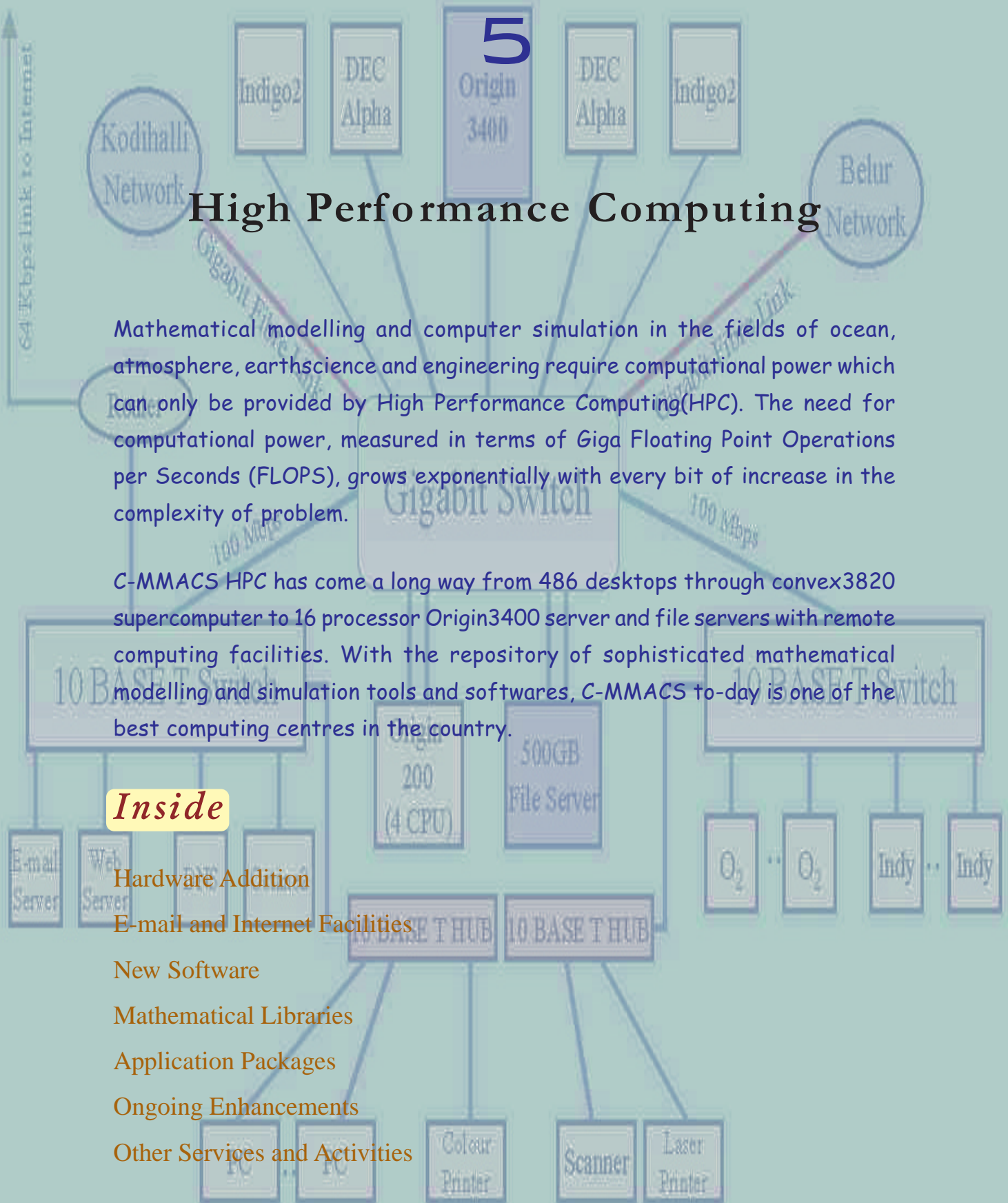
High Performance Computing

Mathematical modelling and computer simulation in the fields of ocean, atmosphere, earthscience and engineering require computational power which can only be provided by High Performance Computing(HPC). The need for computational power, measured in terms of Giga Floating Point Operations per Seconds (FLOPS), grows exponentially with every bit of increase in the complexity of problem.

C-MMACS HPC has come a long way from 486 desktops through convex3820 supercomputer to 16 processor Origin3400 server and file servers with remote computing facilities. With the repository of sophisticated mathematical modelling and simulation tools and softwares, C-MMACS to-day is one of the best computing centres in the country.

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5.1 High Performance Computing

The most significant development that took place during the year 2001-2002 is the procurement and installation of a sixteen processor SGI Origin 3400 server. The machine, one of the most powerful in India, has been successfully installed and commissioned. It consists of 16 R14000 500MHz MIPS processors with 16 GB of main memory. The machine runs with IRIX 6.5 operating system. This machine is expected to boost the Ocean Modelling activities of C-MMACS and other INDOMOD groups. Modular Ocean Model (MOM), Parallel Ocean Program (POP) and Atmospheric Global Circulation Model (AGCM) have been successfully ported on to this new server. IITM Pune uses this machine remotely from Pune. The machine works in parallel mode using both Shared Memory (SHMEM) and Message Passing Interface (MPI). It has checkpoint restart and job queuing facility. It has F77, F90, C and C++ compilers with auto parallel options. Application software like Matlab and CFD-ACE has been made available on this new server.

The existing four processors of SGI Origin 200 server have been upgraded to 360MHz processors from 180 MHz. The operating system of this server was also upgraded from IRIX6.4 to IRIX6.5 along with the compilers. With this upgradation the server will continue to meet the medium level computing requirements of ocean and atmospheric modelling programmes of C-MMACS.

5.2 Hardware Addition

An SGI Octane 2 and O2 workstations were added to the computing environment for scientific visualisation. In order to meet the growing requirement of documenting scientific output at C-MMACS, 2 numbers of HP laser printer with full-duplex printing facility and 5 numbers of HP inkjet printers are added to the CMMACS LAN. Additional 64 MB memory has been added to the existing Compaq Deskpro desktop systems and additional 128 MB memory has been added to IBM Pentium II machines.

5.3 E-mail and Internet Facilities

E-mail services were provided to more than 800 users through C-MMACS mail gateway. The staff members were provided with an alternate connectivity to Internet through the 1Mbps link from NAL Kodihalli campus. A new look C-MMACS website was inaugurated on 1st January 2002 and this website provides information about different activities of the centre. Many links like, on-line books, lecture notes, technical reports, monsoon forecast were newly added to the home page. The site also provides information about recent achievements of C-MMACS as published in various Newspapers. Homepages of NAL and ICAST are also hosted and updated on C-MMACS web server periodically. Information about C-MMACS activities related to Bhuj earthquake is also hosted on this web site.

5.4 New Software

The following software were upgraded (blue) or newly installed (green) during the previous year

- NISA upgraded to version 10.0 on Origin200 server
- CFD-ACE+ upgraded to version 6.6 on IRIX environment.
- GAMIT and GLOBK installed on Origin200 server for earthquake data processing.
- GMT installed on Origin200 for Visualisation
- IDL software installed on Origin 3000 server
- Adobe Publishing Collection
- Microsoft Visual Studio

The table shown below gives the list of available software at C-MMACS in various categories.

5.5 Mathematical Libraries

Package Name	Description	Computing Platform
Complib	High- performance math libraries	SGI
DXML	Extended mathematical libraries	DEC
IMSL	Comprehensive library for numerical and statistical analysis	SGI
NAG	Numerical and statistical analysis	SGI
NUMERICAL	Software for numerical analysis	SGI, Intel
RECIPES		
SCSL	SGI Cray scientific library	SGI

5.6 Application Packages

Biology & Chemistry

AMBER	Modelling of peptides / nucleic acids / carbohydrates	SGI
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
GAMIT	GPS data processing	SGI
GLOBK	GPS data processing	SGI
MOM	Global ocean circulation (Modular model)	SGI
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
NCAR Graphics	Advanced graphics display and mapping	SGI
SigmaPlot	Data manipulation, regression and curve fitting	Intel
SigmaScan Pro	Image digitising software	Intel
TableCurve2D	Automated curve fitting and equation discovery	Intel
TableCurve3D	Automated surface fitting and equation discovery	Intel
TECPLOT	General purpose 3-D graphics	SGI

Structural Mechanics

NISA	Finite element analysis	SGI
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
GNU PLOT	General purpose plotting package	SGI, 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
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

5.7 Ongoing Enhancements

The following procurement have been initiated during the last year and installation are in progress

- Additional one TB disk storage and 7.2 TB tape library for the IBM storage server.
- Purchase order has been placed for the supply of 25 numbers of IBM P4 desktops.
- Phaser860 colour printer.
- Expansion of Local Area Network (LAN)
- Remote Access Server to enable remote computing

5.8 Other Services and Activities

A brainstorming session was organized at C-MMACS on "Quantum Information System and Cryptography as part of CSIR's initiation to identify possible potential research areas where India can take leadership in new millenium. Several researchers and academicians from various research and academic institution in Bangalore have participated in this event.

The campus wide e-mail distribution network was further expanded by adding departmental mail servers in other divisions of NAL. Intel Pentium based servers with LINUX Operating system were installed and configured in ATF and

EAD divisions. These servers are configured with SMTP protocol so that e-mail from users of these divisions will be transferred to C-MMACS mail gateway for instant delivery to its final destination in Internet. Technical assistance was provided to various divisions of NAL to install and configure LINUX and UNIX operating systems for different purposes.

High-end computing and visualization facilities was provided to Ph.D. students from IIT Delhi. In addition, computing resources were provided to the students of various universities through out India enabling them to carry out their academic project works.

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