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Computing Environment

Sophisticated mathematical modelling aided by powerful computing and visualization has the potential to provide the cutting-edge to industry: generation of cost-effective solutions, process optimization and product design are some of the areas where modelling and simulation can play critical to enabling role.

The Industrial Computational Mechanics group at C-MMACS has been utilizing and developing such tools as flow-consistent grid, finite element methods and others to address a wide range of engineering and industrial problems. Several basic results on Finite Element Analyses are reported in his issue.

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5.1 High Performance Computing

The high performance computing facility at C-MMACS which is the lifeline for mathematical modelling and computer simulation in the fields of ocean, atmosphere, earth science and engineering, maintained an uptime efficiency of 100% during the year.

The high performance computing facility at C-MMACS was further enhanced by adding 4 CPU brick with 4 GB memory to the existing sixteen processor SGI Origin3400 server and is currently has 20 R14000 500MHz MIPS processor with 20 GB of main memory. Along with this, the IRIX operating system was also upgraded to version 6.5.19. An additional storage space of 350 GB was added by adding a TP9100 fibre channel RAID system. The machine is being extensively used for ocean modelling activities of C-MMACS and the INDOMOD group of IITM, Pune. In addition, this machine is used by many other academic and research institutions including NAL. This system is mainly used for running models such as Modular Ocean Model (MOM), Parallel Ocean Program (POP), and Atmospheric Global Circulation Model (AGCM) along with application software like IDL, Matlab and CFD-ACE and some of these applications run in parallel mode using Shared Memory (SHMEM) or Message Passing Interface (MPI).

5.2 High Availability File Server

The 500 GB IBM High Availability File Server was upgraded to 1.5 TB, with an addition of one TB disk storage. A new 7.2 TB tape library was installed with automatic backup facility using Tivoli Storage Management (TSM) software.

5.3 Hardware Addition

Twenty five numbers of IBM Netvista A30 desktop computers with Linux/Windows XP Professional operating systems were added to the network. These systems are configured with Pentium 4 @ 1.7 GHz, 256 MB memory, 40 GB hard disk and 17" colour monitor. A 1200 dpi Tektronix Phaser860

colour printer with duplex printing facility, was added to the C-MMACS network for high quality colour outputs.

5.4 E-mail and Internet Facilities

E-mail facility, for about 800 users from e-mail nodes distributed over the campus wide network, is provided through the C-MMACS gateway. Internet facility is provided to C-MMACS users through 64 Kbps connection to ERNET and 1 Mbps link from NAL to VSNL. The C-MMACS website has been made more informative by adding web pages about different activities of the centre and by providing online technical reports and project documents. A web site was created for the ISMMACS Conference on Mathematical Modelling and Computer Simulation, organized jointly by C-MMACS and ISMMACS. Many participants registered through the online facility provided in the web site. Updated information about the conference, such as accepted papers and presentation schedules were provided in the web site. A similar web site has been developed for the International Conference on Scale Interaction on Variabilities of Monsoon (SIVOM), being organised jointly by C-MMACS and Cochin University of Science and Technology to be held at Munnar, Kerala in October 2003. This also provides online registration facility and provides information about the conference venue.

5.5 New Software

The following application software were upgraded during this year.

- A. NISA upgraded to version 11.0
- B. CFD-ACE+ upgraded to version 2002
- C. GAMIT and GLOBK upgraded to version 10.7

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

5.6 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

5.7 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
LMD ACM	Atmospheric General Circulation Model	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
IDL	Interactive data analysis and visualisation	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, Intel

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
FLOWPATH	2-D flow and contaminant transport in sub-surface	Intel
GMT	Generic Mapping Tools	SGI
GNUPLOT	General purpose plotting package	SGI
IDL	Interactive Data Analysis and Visualisation	SGI
MACSYMA	Applied Mathematics software	Intel
MATLAB	Mathematical and symbolic computation	SGI
MathCAD	Mathematical calculation, visualisation and documentation	Intel
MODFLOW	3-D simulation of flow in sub-surface	Intel
PdEase	Applied Mathematics software	Intel
SCILAB	Mathematical and symbolic computation	SGI, Intel
SPSS	Advanced statistical analysis	DEC
TSM	Tivoli storage management software	IBM
Visual MODFLOW	3-D flow and contaminant transport in sub-surface	Intel
Visual Studio	Microsoft Development Tool	Intel

5.8 Ongoing Enhancements

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

- a. Purchase order has been placed for an additional 4 CPU brick with 8 GB main memory for Origin 3400 server.
- b. Expansion of Local Area Network (LAN) to the auxiliary building.
- c. Upgradation of LAN to a high-speed network with gigabit switches.
- d. Remote Access Server to enable remote computing
- e. Upgradation of Matlab and installation of Femlab

5.9 Other Services

Technical assistance was provided to various divisions of NAL for troubleshooting the Linux based E-mail servers. High-end computing and visualization facilities were provided to Ph.D. students from IIT Delhi and Gandhigram Rural Institute. In addition, computing resources were provided to the students of various engineering colleges and universities across the country, enabling them to carry out their academic project works. Technical and computing support were provided for various courses and workshops organised by C-MMACS.

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