

THE COMPUTING ENVIRONMENT

High Performance Computing

Round-the-clock operations on a three-shift basis, of the high performance computing and networking resources of C-MMACS was streamlined during the year 1995-96. A 250 KVA Diesel Generator set was installed and commissioned in November 1995. Consequently, the system availability during 1995-96 increased by 52.06% over the previous year, and the CONVEX utilisation by 50.99% (Table 7). Figs. 23 and 24 show discipline-wise and organisation-wise breakup of the system usage.

Networking

The expansion of the Local Area Network to the first floor of the C-MMACS building has been taken up and it is expected to be operational in mid 1996. The reliability of the leased line connecting C-MMACS to the ERNET node at IISc for Internet connectivity was improved by installing Motorola Codex V.34 SDC modems. A domain name server was setup to improve the Internet services. Netscape Navigator was installed on the Indigo-2 systems and the Web client became operational in September 1995. A radio link has been installed between C-MMACS and ERNET gateway at STP, Bangalore for a robust Internet Connection. This link is currently operational on experimental basis at 9.6 Kbps and its speed will be enhanced to 64 Kbps shortly.

E-mail services were provided to over 160

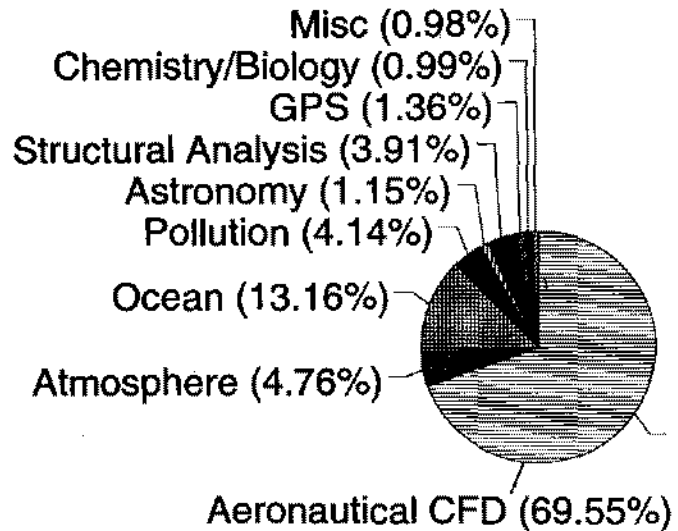


Fig. 23: Discipline-wise breakup of CONVEX utilisation

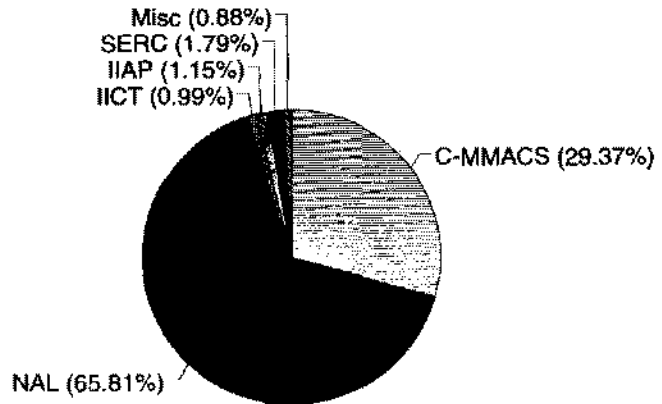


Fig. 24: Institution-wise breakup of CONVEX utilisation

| | 1995-96 | 1994-95 | Change (%) |
|-----------------------|----------|---------|------------|
| Availability (Hours) | 8149.46 | 5359.37 | 52.06 |
| Utilisation (CPU Hrs) | 13590.31 | 9000.52 | 50.99 |

Table 7: Uptime and utilisation of CONVEX C3820

users from C-MMACS and NAL. The services were improved with high speed modems for dial-up lines and mails sent/received using SMTP on the Internet. UUCP connection to C-CADD division of NAL was established for e-mail.

Software

Several software packages including CFD-ACE, CFD-GEOM, CFD-VIEW, PHOENICS, TECPLOT, NAG libraries, MATLAB, GRO-MOS95, etc. were procured and installed on the high performance computing platforms. Table 8 gives the list of software packages.

Other Services

About thirty participants of the course on molecular modelling and drug design were provided hands-on sessions on graphics workstations for five days in October 1995. A two-day Internet course was conducted for over 30 scientists from various CSIR laboratories in March 1996 and live demonstrations were provided on using the World Wide Web.

Ongoing enhancement

Following systems are being procured to further enhance the computing environment.

1. WebFORCE Indy Web Server
2. Ultra Sparc Workstations
3. Indy Workstations
4. Compaq Pentium Servers & Desktops
5. Tektronix Phaser 340P Colour Printer
6. CISCO 2522 router
7. Additional memory for DEC Alpha & Indigo 2 workstations

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Mathematical Libraries

| | | |
|------------|--|-------------------------|
| DXML | Extended mathematical libraries | ALPHA |
| EISPACK | Eigen-system analysis | COSMOS |
| ELLPACK | Solvers for elliptic partial differential equations | CONVEX |
| IMSL | Comprehensive library for numerical and statistical analysis | INDIGO 2, COSMOS, 80x86 |
| ITPACK | Iterative solvers for linear systems | CONVEX, COSMOS |
| LAPACK | Linear algebra | CONVEX |
| LINPACK | Linear system solvers | CONVEX, COSMOS |
| NAG | Numerical and statistical analysis | CONVEX, INDIGO 2, 80x86 |
| ODEPACK | Ordinary differential equation solvers | CONVEX, COSMOS |
| SPARSEPACK | Sparse linear system solvers | CONVEX, COSMOS |
| VECLIB | CONVEX vector libraries | CONVEX |

Application Packages

Biology & Chemistry

| | | |
|----------------|---|---------------------|
| AMBER 4 | Modelling of peptides / nucleic acids / carbohydrates | CONVEX, COSMOS, SUN |
| CHEMKIN | Chemical kinetics | CONVEX, COSMOS |
| GROMOS 95 | Modelling of peptides / nucleic acids / carbohydrates | CONVEX |
| NASACEC | Chemical equilibrium (Combustion) | CONVEX, COSMOS |
| MOPAC 6 | Molecular orbital calculations | CONVEX, COSMOS |
| PCMODEL | Molecular modelling | INDIGO 2, IRIS |
| XPLOR | X-ray crystallographic and solution NMR structure determination | CONVEX |
| CAD/CAE | | |
| AUTOCAD | Computer aided design | 80x86 |
| CAMAND | Computer aided modelling, analysis, numerical control, design and documentation | IRIS |
| CFD-GEOM | Surface modelling and grid generation | INDIGO 2 |
| SDRC I-DEAS | Solid modelling | IRIS |

Table 8: Softwares at C-MMACS (Continued)

Earth Sciences

| | | |
|-----------|--|--------------------|
| BERNESE | GPS data processing | SUN |
| CCM 2 | Community climate model | CONVEX |
| FASCOD 2 | Line-by-line atmospheric radiative transfer | COSMOS |
| LAWPM | Limited area weather prediction | CONVEX, COSMOS |
| LOWTRAN 7 | Atmospheric radiative transfer | CONVEX, COSMOS |
| MOM | Global ocean circulation (Modular model) | CONVEX, ALPHA, SUN |
| TIDAL | Shallow water simulation and pollutant transport | CONVEX, 80x86 |

Fluid Flow, Heat and Mass Transfer

| | | |
|----------|---|---------------|
| CFD-ACE | Computational fluid dynamics | CONVEX |
| NISA | Finite element fluid dynamics code | CONVEX, 80x86 |
| PHOENICS | Computational fluid dynamics | CONVEX, 80x86 |
| PORFLOW | Porous media flow, heat and mass transfer | CONVEX, 80x86 |

Scientific Visualisation

| | | |
|---------------|--|---------------------|
| AVS | Application visualisation system | CONVEX |
| CFD-VIEW | Graphics for CFD | INDIGO 2 |
| GrADS | Graphical display for atmospheric and oceanic applications | INDIGO 2, ALPHA |
| NCAR Graphics | Advanced graphics display and mapping | INDIGO 2, SUN, IRIS |
| TECPLOT | General purpose 3-D graphics | INDIGO 2, 80x86 |

Structural Mechanics

| | | |
|-------------|--------------------------|---------------|
| NISA | Finite element analysis | CONVEX, 80x86 |
| SDRC I-DEAS | Finite element modelling | IRIS |

Table 8: Softwares at C-MMACS (Continued)

Miscellaneous

| | | |
|------------|--|--------------|
| ACRPLOT | General purpose plotting package | 80x86 |
| CSS | Integrated statistical and graphics analysis | 80x86 |
| STATISTICA | | |
| DADISP | Digital signal processing | 80x86 |
| DT-IRIS | Image processing | 80x86 |
| MAPINFO | Desktop mapping | 80x86 |
| MATLAB | Mathematical and symbolic computation | ALPHA, 80x86 |
| NEXPERT | Expert system shell | 80x86 |

Graphics Libraries

| | | |
|--------------|--|----------------------|
| GKS | | INDIGO 2, COSMOS |
| NAG Graphics | | CONVEX, 80x86 |
| OpenGL | | INDIGO 2, ALPHA |
| PHIGS | | INDIGO 2, ALPHA, SUN |

Table 8: Softwares at C-MMACS (*concluded*)