

Annual Report
2004-2005
Centre for Modelling, Simulation and Design (CMSD)

High Performance Computing (HPC) has become an integral part of research and teaching in many branches of study. Along with experiment and theory, computer simulation has become an unavoidable and stabilizing third leg for research activities. The CMSD is conceived to provide such HPC capability not ordinarily available in India and in educational institutions. This was possible with generous support from UGC under “University with Potential for Excellence” programme and from DST under its FIST programme.

CMSD hopes to nurture cross-disciplinary bridges, which are effective in generating new knowledge and creative explorations. The human resources generated from such efforts will be invaluable. Expertise thus developed would help in reaching out to other research organizations and industry. Training individuals and organizations in specific hardware and software, undertaking consultancy and turnkey projects, helping to convert real life questions into appropriate mathematical and computational models are expected outcome. CMSD became operational from its new premises during December 2004.

CMSD HPC is 24 x 7 Facility which is fully networked and consists of the following hardware:

- 5 SMP Systems with total of 192 CPUs [1 x IBM p690 (32 Power 4), 3 x IBM p690 (96 Power 4+), 1 x IBM p595 (64 Power 5)], 384 GBytes of main memory and 4 TBytes of storage,
- A CDAC PARAM SUN cluster consisting of 16 nodes (each with dual xeon processors) and 32 GB memory and
- High end workstations such as 6 x SGI Octone 2, 2 x SUN Blade 2000, 6 x IBM Intellistations etc.

To support various application domain areas following software have been deployed on the above hardware: Accelrys Suite, Gaussian 2003, MOPAC, Relibase+, Molpro, ADF, GCG Wisconsin, SPSS, Mathematica, Statistica, GAMS, RATS, Matlab with various toolboxes, CFX 5.7, 3D Studio Max, iSIGHT Pro, BOS, BEAMPRO etc.

Several researchers from San Diego Supercomputing Centre (USA), Anna University (Chennai), S. N. Bose Institute (Kolkata), IISc (Bangalore), IBM, SUN, CRAY etc have visited the Centre. Further advanced courses, workshops and lectures by leading professionals have been conducted.

At present Prof. Arun Agarwal is Professor-in-Charge of the CMSD. Prior to him Prof. E. D. Jemmis was the Incharge.