

**Annual Report  
2005-2006  
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. Needles to emphasize that the human resources generated with such expertise from such efforts will be invaluable. Thus the primary goals of this facility are directed towards:

- a. developing skills in formulating real life problem as tractable mathematical models that can be solved by state-of-the-art computational methods;
- b. training individual specialists and organization in the latest Hardware and Software, thereby augmenting the technological base in the country and finally;
- c. developing capability to undertake consultancy and execute major projects on turn-key basis.

CMSD became operational from its new premises in December 2004.

Currently, CMSD is a Teraflop 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, GAMESS, SPARTAN 2003, NAG Fortran SMP Library, Empire 3D V4.2, Ansys Multiphysics, AWR (microwave Office), Full Wave Sonnet etc.

Prof. Mark Gahegan, Associate director of GeoVISTA centre, Professor of Geography Pennsylvania State University, was UPE Visiting Professor at CMSD from January 7 to 27, 2006 and Dr. Chaitan Baru, Director R&D, San Diego Supercomputer Centre, UCSD, USA, UPE Visiting Professor at the CMSD from October to December 2005.

Several researchers visited the CMSD like Prof. Gadre, University of Pune, Prof. B. T. N. Sridhar, Anna University; Prof. Balakrishnan, IISc Bangalore, Dr. Sumita Datta, SN Bose National Centre for Basic Sciences, Kolkata, etc.

Further advanced courses, workshops and lectures by leading professionals have been conducted, in particular PRAGMA-9 Workshop on Grid Computing was held during October 21-23, 2005. About 100 delegates participated, including about 50 from abroad and a Geosciences Workshop was held from October 24-27, 2005 in collaboration with SDSC (USA), CESS (UoH, India). Cluster training was conducted by CDAC from January 3-7, 2006. Students from Physics, Chemistry and Computer Sciences participated in the training programme.

Under Distinguish Lecture Series, Prof. Mark N Gahegan, Associate Director of GeoVISTA centre, Professor of Geography, Pennsylvania State University, delivered a lecture on Knowledge Discovery, Visualisation and the process of science, on January 25, 2006

Prof. Arun Agarwal is Professor-in-Charge of the CMSD.