

**Annual Report  
2006-2007  
Centre for Modelling, Simulation and Design (CMSD)**

High Performance Computing facility in CMSD became operational from its new premises in December 2004. However, it was only this year we were able to make the first floor operational. CMSD now offers the following high quality facilities besides the HPC access:

- Two training rooms for 32 and 12 participants
- A Seminar Hall to occupy 95 delegates
- Three discussion rooms each with a capacity of 16 persons
- 13 well equipped (telephone, computer, sofa set etc) office space for visiting faculty/researchers
- A Board Room with VTC facility
- A Visitor's lounge
- A complete wireless access within the building
- A pantry room

Currently, CMSD is a 1.3 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. This year additional softwares were added: Cadence, ISATIS, modules of Accelrys, HPC compilers (like Fortran 90, Intel, Lahey compilers, PGI compilers, Absoft Fortran Compiler etc) on various platforms. Image Processing S/W like ERDUS.

### **Academic Status**

The STAC/AC has recommended academic status to CMSD which will facilitate the Centre to undertake and complete academic programmes as underlined in the Statutes, Objectives of the Centre. The following are the plans:

- a) To support short certified training programmes for students of the campus which will provide incremental values addition skills that would create better job opportunity.
- b) To create Associate Faculty of the CMSD from other Schools and Departments.

### **Allotment of HPC Time**

1. Assessment and feasibility of short range weather prediction for Andhra Pradesh and for Hyderabad city using high resolution numerical models, by Prof. D. V. Bhaskar Rao, Andhra University
2. Quantum Chemical Studies on Amyloid- $\beta$  polypeptide involved in Alzheimer's disease, by Dr E. J. Padma Malar, University of Madras
3. Ocean-Atmospheric Modelling, Dr. V. Sundararajan, CDAC, Pune
4. Dr Y. Soujanya, IICT, Hyderabad
5. Dr. Suresh, RRL Labs
6. Prof. J. B. Joshi
7. Prof. Kolandveil

### **Visitors**

- Prof. D. P. Landau, University of Georgia, USA to visit as a Visiting Professor to CMSD and School of Physics.
- Prof. Turab Lookman, a Computational Physicist from the Los Alamos National Lab, USA, visited during February 1-10, 2007.
- Dr. Sudhakar Pamidighantam, Scientific Computing Division, National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign, USA, visited and gave lecture on "Web Services for Production Cyberenvironment for a Computational Chemistry Grid", on March 17, 2007

### **External Linkages**

A letter of commitment has been issued to the University of California, University of Wisconsin, University of Illinois, Urbana-Champaign and Sandiego Super Computer Centre, USA, to allow their students to visit University of Hyderabad under PRIME project of NDF, USA. They are likely to visit our university for 8-10 weeks. These students will be engaged on the ongoing projects of research being carried out at CMSD.

### **Workshops**

Project Management Board of DST recommended that three HPC workshops be conducted at Hyderabad, Kolkata, and Trichy during February, April and August 2007, respectively. Prof. Arun Agarwal, Dr. G. P. Das and Prof. M. Lakshmanan would coordinate this activity, respectively at each of the three sites. First Workshop was successfully conducted from February 19-22, 2007

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