

## **Centre for Modelling Simulation and Design**

### **PREAMBLE:**

The University of Hyderabad, having expertise in many of the above areas, fully appreciates the inter-dependence of Science, Engineering and Technology, and launched a uniquely conceived new programme. This initiative was launched through an imaginative programme of the UGC (recognizing the University for its Potential for Excellence) by establishing a designated Centre for such activity (Centre for Modelling, Simulation and Design - CMSD). This programme has been receiving generous support from DST under its FIST program.

CMSD aims 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. Training individuals and organizations in specific hardware and software, undertaking of consultancy and turnkey projects, help convert real life phenomena into appropriate mathematical and computational models etc., are some of the important tasks that CMSD has embarked on. This center became operational from its new premises in December 2004.

The study of passage from the micro world of atoms and molecules to the macro world of solids, liquid and gases calls for an understanding of a variety of phenomena in Physics, Chemistry, Biology and Engineering Science and technology and related areas. Atomic lasers, molecular computers, drug-receptor interactions, industrial catalysts, lubricants, and industrially important materials form part of this continuum and an understanding of this evolution needs all the three components of research, viz. theory, experiment and computation. Computer-based simulations now form an integral part of modern research methodology and in this era of science-driven-engineering and directed basic research, the role of scientific research based on modelling, simulation and design, is of paramount importance. The primary requisite in using the third avenue of research for solving complex problems is a working, state-of-the-art High Performance Computing (HPC) center.

One of the unique academic features of this center is that all the active computational scientists working in widely different academic disciplines in the University campus are associate faculty of the CMSD, and contribute their expertise and experience in furthering its objectives. Some of the research interests of these members include: physics of low dimensional systems, topological defects in fluids in restricted geometries, critical phenomena in complex fluids and magnetic systems, Monte Carlo simulations and development of novel sampling techniques, genomics and bioinformatics protein folding, cognitive neuroscience, computational intelligence, natural language understanding, Very Large Scale Integration (VLSI), quantum chemistry and Density Functional Theory (DFT), molecular modeling, drug design and delivery, design of new materials etc.

Currently, CMSD has approximately 25.0 Teraflop Facility which is fully networked and consists of the following hardware:

### **COMPUTATIONAL FACILITY**

- 6 SMP systems with total of 192 CPUs [1 x IBM p690 (32 Power4), 3 x IBM p690 (96 Power4+), 1 x IBM p595 (64 Power5)], 1 x IBM p595 (64 Power5+) @ 2.3 GHz, 512

GBytes of main memory and 4 TBytes of storage.

- A CDAC PARAM SUN cluster consisting of 16 nodes (each with dual Xeon processors) and 32GB memory.
- High end workstation such as 6 x SGI Octane 2, 2 x SUN Blade 2000, 6 x IBM intellistations etc.
- SGI Altix 4700a 128 core (Dual Core, Itanium29150M 1.67 GHz) shared memory architecture based Unix server comprising of 512 GB RAM.
- SGI Altix ICE 8200 EX Cluster [Enhanced] with 1024 core high performance, high throughput and high availability cluster comprising of 1 GB/core memory, built using Infiniband Interconnect.
- SGI XE1300, 2 x Quad core @ 3.0GHz, 8 GB RAM, 146 GB HDDA 128 core Windows CCS/HPC Cluster.
- SGI IS4600 x 2, 100TBytes of shared storage system (FC, SATA) for delivering very demanding data intensive environment, leading to High Performance & Productive Computing Facility, through SGI Altix 450 x 2, 8 core, 48 GB RAM, Montvale 1.67 MHz storage servers.
- SGI Spectra T120 Library, 2 x LTO Gen-4 Drives scalable to 6, Spectralogic 100 slots and 60 units of Media, a good tape backup system to archive data with time stamping.
- Management Servers: SGI Altix 250 SERVER x 10 (2U), 2 x Quad core, E5472, 3.00 GHz 1600 FSB, 12MB Cache, 8GB RAM 6 x 145GB SAS HDD/15K.
- Parallel file system to allow bulk I/O operations.
- 16 No's IBM POWER 7 - 755 Server with total of 512 CPUs - 4 x 8 core 3.3 GHz Power 7 Processor, 2 x 146 GB DASD 128 GB DDR3 RAM.
- IBM storeWize V7000 based Storage with 60TB RAW Storage Capacity (30 x 2TB Disks)
- An integrated linux cluster system with 1.0 TeraFlops computing power having all open source compiler and software for training and executing home grown codes.
  - To support various application domain areas the following software are deployed on the above hardware: Accelrys suite, Gaussian 2003, MOPAC, Relibase+.
  - Molpro, ADF, GCG Wisconsin, SPSS, Mathematica, Statistica, GAMS, RATS, Matlab with 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, ArcGIS, ArcMIS, Cadence, ISATIS, TURBOMOL, Image Processing S/W like ERDUS, LABVIEW, Keil etc.

## **VISUALIZATION FACILITY**

- NVIDIA Quadro FX 5600 Active Stereo Graphics Card
- Windows XP Professional o 750GB SATA Disk Drives
- 22" LCD Monitor • SGI Image generator – VN200 system,
- DVD Drive, 2xGbE Ethernet,

- Two quad-core Intel Xeon E5462 2.8GHz processors
- 16GB DDR2 800 REG ECC Memory
- NVIDIA Quadro FX 5600 Active Stereo Graphics Card
- SLES 10 Linux o 160GB SATA Disk Drives
- 22” LCD Monitor
- Christie Mirage HD6 3chip stereo DLP projector and Lens
- Screen - 9ft x 6ft fabric
- Crosspoint 450 Plus 84HVA Matrix Switcher RGB for video & Stereo Audio
- Video and Audio interface – Extron RGB 109
- Audio Amplifier
- NuVision Active Stereo Glasses
- Nuvision Stereo Emitters (mid-range)
- Wireless AMX control system
- CEI Ensign Application Software
- Remote Visualization Software Single User

**Professor-in-Charge : Prof. Chakravarthy Bhagvati**