

**Annual Report
2010-2011
Centre for Modelling Simulation and Design (CMSD)**

PREAMBLE

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, 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 modeling, 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.

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 of higher education and research. 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 Centre became operational from its new premises in December 2004, and is now launching its academic programmes.

One of the unique academic features of this Centre 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 academic 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, Molecular modeling, Drug design and delivery, Design of new materials etc

Currently, CMSD has a 15.0 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 Power 4), 3 x IBM p690 (96 Power 4+), 1 x IBM p595 (64 Power 5)], 1 x IBM p595 (64 Power 5+) @ 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 32 GB memory.
- High end workstations such as 6 x SGI Octone 2, 2 x SUN Blade 2000, 6 x IBM Intellistations etc.
- SGI Altix 4700 a 128 core (Dual Core, Itanium2 9150M 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, 4 GB RAM, 146 GB HDDA 128 core Windows CCS/HPC Cluster.
- SGI IS4600 x 2, 100 TBytes 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 x9 (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.

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, etc.

VISUALIZATION FACILITY

- NVIDIA Quadro FX 5600 Active Stereo Graphics Card
 - Windows XP Professional
 - 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
 - SLES10 Linux
 - 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 RGB109
- Audio Amplifier
- NuVision Active Stereo Glasses
- NuVision Stereo Emitters (mid range)
- Wireless AMX control system
- CEI Ensign Application Software
- Remote Visualization Software Single User

Adjunct Professor

1. Prof. Claudio Zannoni, Dipartimento di Chimica Fisica Ed Inorganica, Universita di Bologna, Italy, (February 18, 2009 to February 17, 2011).
2. Prof. Anil Kumar, Dept. of Physics & NMR Research Centre, Indian Institute of Science (June 20, 2009 to June 19, 2012)

Visiting Professor

1. Dr. Debasis Chakraborty, Scientist 'G', Directorate of Computational Dynamics, DRDL, Hyderabad
2. Dr. M R Reddy, Metabasis Therapeutics, San Diego, USA.
3. Dr. Ingua Ramarao, Computational Physicist, East West Enterprises Inc., USA

Post-Doctoral Fellow

Dr (Ms) G. Sai Preeti, recipient of UGC Dr. D. S. Kothari Postdoctoral Fellowship has joined CMSD on February 2011, for a period of 3 years. She previously worked as a Post doctoral research assistant in the Dipartimento di Chimica Fisica ed Inorganica, Università di Bologna, funded by the European Council project 'BIND' after obtaining her PhD from University of Hyderabad.

Workshops Conducted

1. Department of Computer & Information Sciences, ACRHEM Jointly organised Colloquium on Computational Intelligence (Rough Set based approach) during March 23-24, 2010 at University of Hyderabad.
2. Department of Meteorology and Oceanography, Andhra University Jointly Conducted a Work Shop on ATMOSPHERIC MODELING FOR WEATHER AND CLIMATE STUDIES during June 23 - July 2, 2010 at Andhra University, Visakhapatnam.
3. IIT Kharagpur Jointly Conducted a Work Shop on Oceanographic Processes and its Modeling of Weather & Climate during July 5-16, 2010 at IIT Kharagpur.
4. Conducted a Work Shop on MOLECULAR MODELLING and DRUG DESIGN during August 2-7, 2010 at University of Hyderabad.
5. Madurai Kamaraj University Jointly Conducted a Work Shop and Conference on Monte Carlo Simulation during August 9-13, 2010 at School of Physics, Madurai Kamaraj University.
6. Advanced Centre for Research in High Energy Materials Jointly Conducted a Work Shop on COMPUTATIONAL FLUID DYNAMICS during September 21-25, 2010 at CMSD, University of Hyderabad.
7. Centre for Nonlinear Dynamics, Bharathidasan University Jointly Conducted a Work Shop and Conference on COMPUTATIONAL METHODS for NONLINEAR DYNAMICS during September 22-25, 2010 at Centre for Nonlinear Dynamics, Bharathidasan University.
8. Conducted a Work Shop on MATERIAL MODELLING AND SIMULATION, during December 27-31, 2010 at CMSD, University of Hyderabad.
9. Anna University, MIT Campus, Chennai Jointly Conducted a Work Shop on Grid Computing during February 7-11, 2011 at Department of Computer Technology, MIT Campus, Anna University.
10. Mizoram University Jointly Conducted a Work Shop on Computational Physics during February 14-19, 2011 at Department of Physics, Mizoram University.

Research Collaboration

PRIME is a unique program which provides undergraduates with hands-on, full-time research experiences in internationally collaborative settings. Against the backdrop of living abroad in another culture, the students work as full-time researchers in one of 13 host institutions in Australia, China, India, Japan, Malaysia, New Zealand and Taiwan, working closely with mentors at both their host institution and back at UC San Diego.

Two undergraduate students of University of California, San Diego (UCSD) in the Pacific Rim Undergraduate Experiences (PRIME) program -- 33 -- visited University on a nine-week summer work (June 23 to August 23, 2010):

The following two are the PRIME students selected by UCSD and spent time for nine weeks in CMSD.

Name of the Student	UCSD Mentor	UoH Mentor
Lee, Keith	Tilak, Sameer	Agarwal, Arun
Wingfield, Raymond	Tilak, Sameer	Agarwal, Arun

Training

1. Centre for Development of Advanced Computing Jointly Conducted a training cum workshop on GARUDA Boot Camp during November 23-24, 2010 at CMSD, University of Hyderabad.

Papers Published

1. T. Mondal and S. Mahapatra, Photo physics of fluorinated benzene. I. Quantum chemistry, *J. Chem. Phys.* **133**, (8), 084304 (2010)
2. T. Mondal and S. Mahapatra, Photo physics of fluorinated benzene. II. Quantum dynamics, *J. Chem. Phys.* **133**, (8), 084305 (2010)
3. D. Jayasri, Regina Jose, K. P. N. Murthy and V. S. S. Sastry, Nematic liquid crystals in contact with geometrically and chemically patterned substrates: A Monte Carlo study, *arXiv:1010.3106* (2010)
4. P. Ravi, G.M. Gore, Surya P. Tewari and A.K. Sikder, Quantum chemical studies on the fused nitro azoles, *Journal of Molecular Structure* , 955(1-3), 171-177, (2010)

5. P. Ravi, G.M. Gore, V. Venkatesan, Surya P. Tewari and A.K. Sikder, Theoretical studies on the structure and detonation properties of amino-, methyl-, and nitro-substituted 3, 4, 5-trinitro-1*H*-pyrazoles, *Journal of Hazardous Materials*, 183, (1-39), 2010, 859-865
6. P. Ravi, G.M. Gore, Surya P. Tewari and A.K. Sikder, Quantum chemical studies on the condensed polynitroazoles, *Journal of Molecular Structure: THEOCHEM* 958, (1-3), 2010, 52-58
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10. Aparoy, P.; Reddy, R.N.; Guruprasad, Lalitha; Reddanna, P, Computational Analysis of Interactions of Argadin with Chitotriosidase, Chitinase and Acidic Mammalian Chitinase: Hints for Specific Inhibitor Design, *Letters in Drug Design & Discovery*, **7**, (5), 2010, pp. 324-331(8)
11. Prasad, Dasari L. V. K.; Jemmis, Eluvathingal D.; Stuffed Fullerene like boron carbide nano clusters, *Applied Physics Letters* **96**, (2), 023108 - 023108-3, (2010)
12. Lavanya Kundu, S C R Roshan, B K Latha, K P N Murthy, and V S S Sastry, Polymer network induced order in biaxial nematic liquid crystals: A Monte Carlo Study, *Solid State Physics (India)* 55 (2010)
13. B. K. Kuntal, P. Aparoy, P. Reddanna, EasyModeller: A graphical interface to MODELLER, *BMC Research Notes* 3, 226 (2010).
14. B. Sudhamalla, M. Gokara, N. Ahalawat, D. G. Amooru, and R. Subramanyam, Molecular Dynamics Simulation and Binding Studies of β -Sitosterol with Human Serum Albumin and Its Biological Relevance, *J. Phys. Chem. B* 114, 9054 (2010).

15. M. Gokara, B. Sudhamalla, D. G. Amooru, R. Subramanyam, Molecular Interaction Studies of Trimethoxy Flavone with Human Serum Albumin, PLoS ONE, 5, e8834 (2010).
16. A. R. Biju and M. V. Rajasekharan, $[\text{Mn}(\text{acac})_2(\text{HOCH}_3)_2]_3[\text{Ce}(\text{NO}_3)_6]$; Icosahedral Anion Builds a Cubic Network, Crystal Growth & Design, 10, 426 (2010).
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21. S C R Roshan, Lavanya Kundu, Regina Jose, K P N Murthy, and V S S Sastry, Azimuthal bistability in patterned Nematic Liquid Crystal Films: A Monte Carlo study, Solid State Physics (India) 55 (2010)
22. Hima Bindu Kolli, Ch Sandhya, V S S Sastry and K P N Murthy, Phase Transition in a Bond-Fluctuating Lattice Polymer, Solid State Physics (India) 55, (2010)
23. Polamarasetty Aparoy, Bhusan Kumar Kuntal and Pallu Reddanna, Development of Tools and Database for Analysis of Metal Binding Sites in Protein, Protein & Peptide Letters, 2010, 17, 000-000
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- the Structure and Bonding of Metallacyclocumulenes, - Cyclopentynes and - cycloallenes, *Organometallics*, 2011, 30 (10), pp 2670–2679
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Prof. Arun Agarwal is the Director of the CMSD. Prof. K P N Murthy and Prof. V S S Sastry are Academic and Resource Coordinators respectively.