

**Annual Report
2007-2008
Centre for Modelling Simulation and Design (CMSD)**

Currently, CMSD is a 2.0 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,
- Last footprint of IBM p595 (64 Power 5+) @ 2.3 GHz with 128 GB RAM has been received and is installed. It was launched by Dr. T. Ramasami, Secretary DST on December 16, 2007.
- 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: ArcGIS, ArcMIS, Cadence, ISATIS, modules of Accelrys, TURBOMOL, 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. A list of approved associate faculty is attached.

Prof. K. P. N. Murthy, has a Joint appointment with CMSD and School of Physics. He is the Coordinator (Academic Affairs) for CMSD and would report to Professor-in-Charge.

Alottment of HPC Time

a. Proposals received and permitted to use (External):

- i. Sambhu. N. Datta, Department of Chemistry, IITB, “Theoretical and Computational Study of Magnetic Properties of Organic Diradicals and Transition Metal Complex in Molecular Crystals”.
- ii. Prof. Shridhar Gadre, Department of Chemistry University of Pune, “Application Of Molecular Tailoring Approach For Geometry Optimization Of Large Molecules And Clusters”.
- iii. Dr. B. T. N. Sridhar, Center for Aerospace research MIT, Anna University Campus, “Hypersonic Flow Simulations”.
- iv. Prof. Balasubramanian Sundaram, JNCASR, Bangalore, “ Ab initio molecular dynamics study of 1-n-butyl-3-methylimidazolium hexafluorophosphate and carbon dioxide mixture.
- v. Prof. E. D. Jemmis, IISc, Bangalore
- vi. Prof. D. V. Bhaskar Rao, Andhra University, “Assessment and feasibility of short range weather prediction for Andhra Pradesh and for Hyderabad city using high resolution numerical models”
- vii. Dr E. J. Padma Malar, University of Madras, “Quantum Chemical Studies on Amyloid- β polypeptide involved in Alzheimer’s disease”
- viii. Prof. P. Kolandaivel, Department of Physics Bharathiar University Coimbatore, “Structure And Characterizations Of Biological Ion Channels In Bio Membranes”.
- ix. Prof. S. Pardasathy, Bharathiar University Coimbatore
- x. Dr. R. B. Sunoj, IIT Bombay
- xi. Prof. G. P. Das, Kolkata
- xii. Dr. Jayant K Singh, IIT Kanpur
- xiii. Dr. Subhash V. Ghaisas, University of Pune
- xiv. Dr. S. B. Sharma, “Toxicity Studies”, Department of BioChemistry, College of Medical Sciences, Delhi
- xv. Mr. M. V. Maheshkumar, JRF, Department of Applied Chemistry, CUSAT, "Theoretical Designing of Donor-Acceptor type conjugated polymers for Optoelectronics”
- xvi. Professor Shankar Prasad Das, School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110067, India

b. Other than FIST Centres

- i. Dr. V. Sundararajan, an established scientist in CDAC, Pune working in the area of Ocean-Atmospheric Modelling.

- ii. Dr Y. Soujanya, a promising scientist of ICT, Hyderabad for her work to model the mechanism of interaction of P450 with its substrate.
- iii. Dr. Cherumuttathu H. Suresh, Regional Research Laboratory – CSIR, Trivandrum
- iv. Dr. Sumita Dutta S.N. Bose National Centre for Basic Sciences, Kolkata, “Simulations Of New Monte Carlo Methods For Generating Random Numbers”.
- v. Dr. Ravichandran, Scientist, Indian National Centre for Ocean Information Services, Hyderabad, “Study Upper Ocean Thermohaline Structure Of North Indian Ocean On Intra-Seasonal And Inter-Annual Time Scale”.

Visitors

1. Sri Rajeev Kapri of Institute of Physics, Bhubaneshwar visited the CMSD for one week during July 15-22, 07. He worked on zipping transition in DNA.
2. Mr. Jayanth and Miss. Padma, Chennai Mathematical Institute, Chennai from 11 - 17, July, 2007. They worked under supervision of Prof. K P N Murthy on a problem in non-equilibrium statistical mechanics.
3. Three scientists from BARC, Amit Thakur, Anek Kumar and Amod Mallick., Mumbai visited from August 2 to 16, 2007 to discuss on a variety of computational and computer simulation problems in reactor core, reactor blankets and reactor shields.
4. Dr. Tilak Agrewala, Vice-President Research, IBM, USA, August 9, 2007.
5. Prof. Artur Baumgaertner, Staff Member, Institut fuer Festkoerperforschung Forschungszentrum Julich, Germany, November – December 2007.
6. Dr. Tilak Agrewala, Vice-President Research, IBM, August 9, 2007.
7. Prof. Dr. G. Ananthakrishna, Raja Ramanna Professor, Materials Research Centre, IISc, Bangalore. From November 15 to 31, 2007.
8. Prof. S. V. M Satyanarayana, Department of Physics, Pondicherry University, Pondicherry
9. Dr. S. L. Narasimhan, Solid State Physics Group, BARC
10. Prof. Dr. Hans C. Fogedby a statistical mechanics and condensed matter physicist of international repute. Presently a professor at the Department of Physics and Astronomy, University of Aarhus, Denmark from January 2008

Workshops

1. Project Management Board of DST recommended that three HPC workshops be conducted at Hyderabad, Kolkata, and Trichy during February, April and August 2007, respectively. Advertisement was prepared and brought out in the three issues of the Current Science. Prof. Arun Agarwal, Dr. G. P. Das and Prof. M. Lakshmanan would coordinate this activity, respectively at each of the three sites.

- a. First Workshop was successfully conducted from February 19-22, 2007 in CMSD, University of Hyderabad
 - b. Second Workshop conducted from April 23-26, 2007, in IACS, Kolkata
 - c. Third Workshop conducted from August 3-6, 2007, in Bharathidasan University, Tiruchirapalli.
2. Accelrys Materials Studio Software Workshop was held from July 26-27, 2007 with Accelrys at CMSD, University of Hyderabad.
3. GEON Workshop held from August 3-8, 2007 at CMSD
 - a. US Resource Scientist
 - i. Dr. Chaitan Baru, SDSC
 - ii. Mr. Ashraf Memon, SDSC
 - iii. Mr. Sandeep Kumar, SDSC
 - b. Indian Resource Scientist
 - i. Dr. K. Radhakrishnan and S.K. Subramanian, NRSA
 - ii. Dr. V P Dimri and Dr. H. V. Rambabu, NGRI
 - iii. Dr. Shailesh Nayak, Dr. M. Ravi Chandran, INCOIS
 - iv. Dr. J. Saibaba and Mrs Lakshmi, ADRIN
 - v. Dr. K. Mruthyunjaya Reddy, Dr. V Raghu and Mehar Baba, APSRAC
 - vi. Dr. Manish Gupta, IBM
 - vii. Mr. Rajesh Chhabra, Altair, Bangalore
 - viii. Prof. K. V. Subbarao, Prof. Arun Agarwal and Dr. Rajeev Wankar, UoH
4. Organized a lecture series on "Simulations in Biology and Soft Matter" from 26th November to 11th December 2007. Following external experts delivered the lectures:
 - i. Prof. Dr. G. Ananthakrishna, Raja Ramanna Professor, Materials Research Centre, IISc, Bangalore.
 - ii. Prof. Artur Baumgaertner, Staff Member, Institut fuer Festkoerperforschung Forschungszentrum Julich, Germany
 - iii. Prof. S. V. M Satyanarayana, Department of Physics, Pondicherry University, Pondicherry
 - iv. Dr. S. L. Narasimhan, Solid State Physics Group, BARC

Internal speakers were: Prof. V S S Sastry, Dr. Janaki Balakrishnan, Dr. B. Ashok, Prof. K. P. N. Murthy

5. Organized a lecture series on "Simulations of Phenomena in Biological Systems and Soft Matter" from 26th November to 11th December 2007. Following external experts delivered the lectures: Prof. A Baumgaertner, Prof. G. Ananthakishna, Prof. S. V. M Satyanarayana and Dr. S. L. Narasimhan.

6. Instructional workshop on Bioinformatics, during December 16-19, 2007 by Centre for Biotechnology of School of Life Sciences, CMSD, and CR Rao Advanced Institute of Mathematics, Statistics and Computer Science (CRAIMSCS).
7. Accelrys Material Studio Workshop, conducted by Dr. Amit Kulkarni, on January 10, 2008.
8. Accelrys Discovery Studio Workshop: Protein Homology Modelling, conducted by Jeff Nauss, on January 31 and February 1, 2008.
9. Multicore Programming Workshop by CMSD and CDAC from February 5 to 9, 2008.
10. Mr. Y. V. Rao, Director, Systems Technology Group, CISCO, March 15, 2008 gave a talk on "Self-Defending Networks".
11. Joint Workshop between University of Hyderabad, IIIT-Hyderabad and Waseda University (Tokyo, Japan), from March 10-11, 2008

Projects Submitted

1. Grid Fabric/Middleware Technologies for Developing Framework for Deploying Ocean Related Applications and Services, awarded by INCOIS, Hyderabad. (With UCESS, DCIS). 60 Lakhs sanctioned, with Professor Arun Agarwal as the PI.

Prof. Arun Agarwal is the Director of the CMSD.