Annual Report
2009-2010
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:

- 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.

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.

Upgrade in Pipeline

- A large SGI 128 core shared memory architecture based Unix server comprising of 4GB/core memory.
- A large SGI Altix ICE cluster with 1024 core high performance, high throughput and high availability cluster comprising of 2 GB/core memory, built using Infiniband Interconnect.
- A 100 TBytes of shared Storage system (FC, SATA) for delivering very demanding data intensive environment, leading to High Performance & Productive Computing Facility.
- Parallel file system to allow bulk I/O operations.
- A good tape backup system to archive data with time stamping.
- A 128 core Windows CCS/HPC Cluster.

The above systems (with 15 TFlops capabilities) are to be seamlessly integrated with the existing resources in the CMSD.

Adjunct Professor

1. Prof. Claudio Zannoni, Dipartimento di Chimica Fisica Ed Inorganica, Universita di Bologna, Italy, (February 18, 2009 to February 17, 2011). Visited from December 3 – 12, 2009.
2. Prof. Anil Kumar, Dept. of Physics & NMR Research Centre, Indian Institute of Science (June 20, 2009 to June 19, 2012)

Visiting Professor

1. Professor Paolo Pasini, Professor of Physics, University of Bologna, Italy (December 3 – 12, 2009)
2. Dr. Debasis Chakraborty, Scientist 'G', Directorate of Computational Dynamics, DRDL, Hyderabad
3. Dr. M R Reddy, Metabasis Therapeutics, San Diego, USA.

Visitors

1. Dr. Ingua Ramarao, Computational Physicist, East West Enterprises Inc., USA, September 16-18, 2009

Seminars

1. Dr Ram D. Sriram, "Systems Biology and Medicine" National Institute of Standards and Technology, USA; August 26, 2009
2. Prof. Claudio Zannoni, "Computer Simulation of Liquid Crystals and Other Soft Matter Systems", Dipartimento di Chimica Fisica Ed Inorganica, Universita di Bologna, Italy; December 10, 2009.

Workshops

1. Conducted HPC workshop on "NVIDIA Tesla Supercomputing Workshop" on July 30, 2009. Jointly sponsored by NVIDIA and Connoiseur Electronics Pvt. Ltd. 75 participants attended the workshop.
2. SPSS South Asia, Bangalore conducted a workshop on PASW Modeler-A Data Mining Workbench, on August 14, 2009
3. The Cloud Computing workshop (December 21 to 23, 2009) provided the participants with an understanding on the fundamentals, deployment and application architecture & design of the fast-growing field of Cloud computing. To provide the most current and complete information, University of Hyderabad and IEEE Hyderabad Section had co-organized this dynamic new field of technology! 83 participants participated in the workshop, of which 50% were students, 20% faculty from colleges and 30% from industry. Following were the title and speakers:

a. Cloud Computing: Vision, Hype, and Reality, Rajkumar Buyya, Melbourne University
b. Service Oriented Architecture: Rajeev Wankar, UoH
c. SOAP, JINI, CORBA: Thamarai Selvi, Anna University
d. Virtualization: Murali VN Sappa, IBM
e. Cloud Computing Architecture: Ameeta Roy, IBM
f. Data in the Cloud: Cloud Computing and Data Intensive Applications, Arun Agarwal, UoH
g. Challenges of Cloud Computing: Rajesh Chhabra, Altair Engineering, Inc
h. Cloud Computing Deployment-I: Web 2.0, Apache Tomcat, Google App Engine, Eucalyptus and Map Reduce: Ameeta Roy, IBM
i. Cloud Computing Deployment-II: Virtual Computing Laboratory, J. Srinivas, IBM
j. Cloud Computing Platform and Application: Aneka Cloud Computing: Rajkumar Buyya and Murali Sathya, Manjrasoft Pty Ltd, Australia

4. **Colloquium on Computational Intelligence (Rough Set based approach) March 23rd-24th, 2010**

Objectives of the colloquium was to train in foundations of Rough Sets, to provide skills of Rough Sets & Computational Intelligence and to highlight the importance of Computational Intelligence and Rough Sets in Research and its application in several application domains requiring High Performance Computing.

The colloquium focuses on giving the basics of Computational Intelligence with emphasis on Rough Sets. Participants will understand the basic mathematical and computational foundations of Rough Sets. The colloquium will provide a platform for the participants to interact with domain experts and will be exposed to the current research challenges in Computational Intelligence and Rough Sets. There were about 35 research participants and was well appreciated. During the colloquium Indian Society for Rough Sets (ISRS) was formed.

Recognition

a. G. Sai Preeti, a PhD student from School of Physics, under Prof. V.S.S.Sastry and also DST HPC fellowship holder, received PDF to work with Prof. Claudio Zannoni, Dipartimento di Chimica Fisica Ed Inorganica, Universita di Bologna, Italy.
b. D Jayasri, a PhD student from School of Physics, under Prof. V.S.S.Sastry and also DST HPC fellowship holder, received PDF to work with Professor Slobodan Zumer, Department of Physics University of Ljubljana Jadranska 19SI-1000 Ljubljana SLOVENIA.

Research Collaboration

Three 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 adventure (June 23 to August 23, 2009): working as researchers in CMSD. Photograph below shows them meeting the Vice-Chancellor on August 12, 2009.

Vice-Chancellor Dr. Seyed E. Hasnain is seen with Pro Vice-Chancellor Dr. P C Sarangi including (on his right) are the three PRIME Mentors: Prof. Arun Agarwal, Prof. K V Subba Rao and Prof. Anand K. Kondapi, and (to his left) are three PRIME students: Matthew Mui, Brian McMahon and Dee Chen.

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.

The PRIME students worked on projects in range of areas including engineering, biological, physical and computer sciences. A brief summary of each of their projects follows.

Mentor/s: Host UCSD Mentor	PRIME student, *major* and project summary
	Dee Chen, *bioengineering*
Mentors: Arun Agarwal and Anand K. Kondapi UCSD: Jason Haga	Goal is to screen other members of the DSP family that ensure the inhibitors found from the SSH-2 screen are specific for SSH-2, using DOCK6 installed on the PRAMA grid sites.
	Brian McMahon, *computer science*
Mentors: Arun Agarwal and K V Subba Rao UCSD: Tony Fountain	His project was to set up a data streaming system for a sensor network in the Bay of Bengal. This system will be used to allow near real-time access to data for researchers to study, and possibly predict tsunami activity utilizing DataTurbine software.
	Matthew Mui, *bioengineering: premed*
Mentors: Arun Agarwal and Anand K. Kondapi UCSD: Jason Haga	The goal of the project is to find a specific inhibitor for a dual specificity phosphatase called SSH-2 using the Pragma Grid.

Book Published

1. Prof. K. P. N. Murthy, Excursions in Thermodynamics Statistical Mechanics, Universities Press, Hyderguda, Hyderabad 2008

Training

1. Training Programme on Critical Aspects of Service Rules with focus on VI Pay Commission Recommendations" for the University Employees was conducted by Masters' Institute of Learning and Sharing, Bangalore during September 1-4, 2008, at CMSD
2. CMSD Conducted a training programme on the software "Advanced Design System" (ADS) of Agilent on 24th January 2009.
3. Research Methodology Course" was Conducted in CMSD by School of Social Sciences & Indian Council of Social Science Research, Southern Regional Centre, Hyderabad during 16th February to 2nd March 2009.

Prof. Arun Agarwal is the Director of the CMSD.