



CREATE . INNOVATE . COLLABORATE

Igniting Minds



Centre for Modelling Simulation and Design

University of Hyderabad, India



About the University

University of Hyderabad is a premier institute of post-graduate teaching and research, established by an Act of the Parliament of India in 1974 as a Central University. Over the years, University of Hyderabad has emerged as a top ranking institute of higher education and research in India. The University is located about 20 KMs from the city of Hyderabad on the old Hyderabad-Bombay highway. Stretching over nearly 2300 acres of land, the sprawling, scenic, serene campus is the home of a variety of birds. The University also has a city campus - The Golden Threshold - the residence of the late Sarojini Naidu.

The “objects of the University” as envisaged in the Act are: “to disseminate and advance knowledge by providing instructional and research facilities in such branches of learning as it may deem fit and by the example of its corporate life, and in particular to make special provisions for integrated courses in humanities and science in the educational programmes of the University and to take appropriate measures for promoting inter-disciplinary studies and research in the University.”

University has 8 Schools, 15 Departments and 10 Centres as part of its Academic Programmes, and has other support structures like Library, Central Instruments Laboratory, Central Workshop, Computer Centre, Central Network Facility etc.



Recognition

- University of Hyderabad, was accredited by the National Assessment and Accreditation Council (NAAC) with a rating of five stars for a period of five years.
- University of Hyderabad has been chosen by UGC as “University with Potential for Excellence”.
- The University has also been rated by NISSAT (National Information System for Science and Technology) of the Department of Scientific and Industrial Research (DSIR), Government of India, as the only University under the High Output - High Impact category among the top 50 institutions in India with publications in citation - index journals.
- Many Schools are UGC-(SAP, COSIST) funded and All Science Schools/Departments are DST-FIST Sponsored.

DST National High Performance Computing Facility

at

University of Hyderabad

Centre for Modelling Simulation and Design





CMSD building



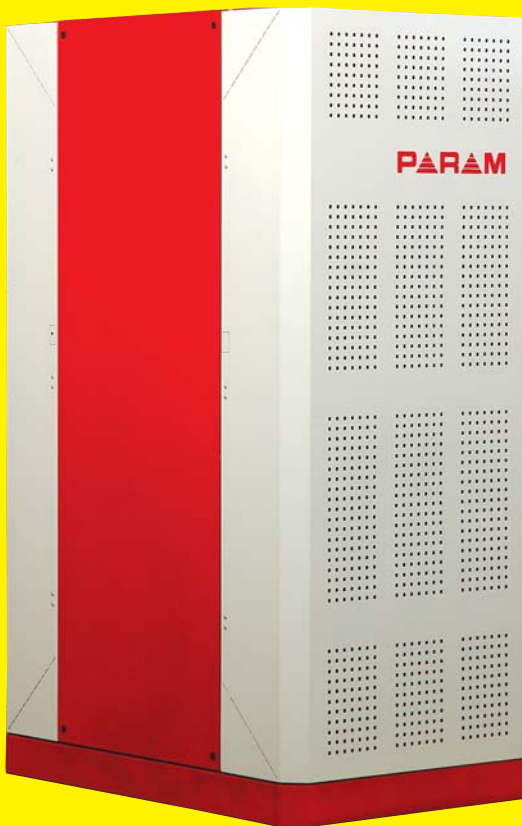
Centre for Modelling Simulation and Design (CMSD)

The passage from atom, molecule, and nanoparticle to bulk matter has emerged as the natural continuum requiring fundamental understanding based on Physics, Chemistry and Biology. 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. Thus computer-based simulations form an integral part of modern research methodology. For example, the design of the best carbon particle size in Tribology involves as much computing as basic science and engineering. In this era of science-driven-engineering, the role of scientific research, based on modeling, simulation and design, is of paramount importance. Countries and Institutions across the world are gearing up to avail the challenging opportunities provided by this new tool. 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 has launched a uniquely conceived new programme of higher education and research. The need for computation in all areas of research and teaching at the University had been felt for long. This initiative has been supported by an imaginative programme of the UGC in recognizing some Universities for their potential for excellence. Of the five Universities selected so far under the scheme, the University of Hyderabad has already proposed, and got approval for, an innovative interfacial studies and research programme with a substantial funding. The UGC approved establishment of the Center for Modeling, Simulation and Design (CMSD) which was fuelled further by generous support from DST under its FIST programme.

CMSD hopes 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. Expertise thus developed would help in reaching out to other research organizations and industry. Training individuals and organizations in specific hardware and software, undertaking consultancy and turnkey projects, helping to convert real life questions into appropriate mathematical and computational models are expected outcome. CMSD became operational from its new premises during December 2004. CMSD has been accorded an Academic Status by the University and Department of Science & Technology recognized CMSD as National High Performance Computing Facility.

Currently, CMSD is a 2 TFlops computing facility and the present demand expects this facility to grow to a 7 TFlops, by positioning an appropriate facility.



Indian High Performance Computing (HPC) System



Computational Resources

Funded by UGC

- 1 IBM SMP p690 System with 32 CPUs (Power 4), with 64GB of Main memory and 400 Gbytes of HDD with 400 Gbytes backup system
- A CDAC PARAM SUN cluster consisting of 16 nodes (each with dual xeon dual core processors) and 32 GB memory
- High end workstations such as 6 x SGI Octane 2, 2 x SUN Blade 2000

Funded by DST

- 3 x IBM p690 (96 Power 4+)+1 x IBM p595 (64 Power 5)+1xIBM p595 (64 Power 5+), 448 GBytes of Main memory and 4 Tbytes of storage with 4Tbytes backup system.
- 6 x IBM Intellistations, with about 100 PCs etc.

Softwares

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, Cadence, ISATIS, HPC compilers (like Fortran 90, Intel, Lahey compilers, PGI compilers, Absoft Fortran Compiler etc) on various platforms, Image Processing s/w like ERDUS.



Research Areas

- VHDL implementation of ID discrete wavelet transform, Programmable universal timer, adaptive PID controller, telecommunication switch etc.
- Non-Boltzman sampling methods to study critical effects in the presence of randomly quenched disorder
- Monte - Carlo Simulation
- Mie scattering from systems of bispheres and cluster of spheres
- Study of Grid Fabric/Middle ware technology
- Computer Aided Drug Design
- Processing, analysis, and calculation of NMR (Nuclear Magnetic Resonance) spectra
- The reactive scattering dynamics of H+HLi collisions
- Model molecular complexation phenomena at the air - water interface
- Sequence and structural analysis of the proteins from *Mycobacterium tuberculosis* genome
- Effect of high pressure on electronic properties of atoms and molecules
- Theoretical study to understand Reaction of aroyl hydrazones with β - diketones in 2:1 ratio
- Design of molecular structures of theoretical and practical importance
- Modelling of Human Topoisomerase II
- Mapping and identification of genomic regions (Quantitative Trait Loci) associated with drought tolerance in rice
- Homology Modeling of Cyclooxygenase -3 (COX - 3)
- Modelling of insect hexamines and their receptors



Integrating Earth Sciences and Technology

Oil Exploration, Seismic Reservoir Monitoring,
Simulation & Modelling



Atmospheric Sciences

Monsoon Forecasting, Simulation & Modelling

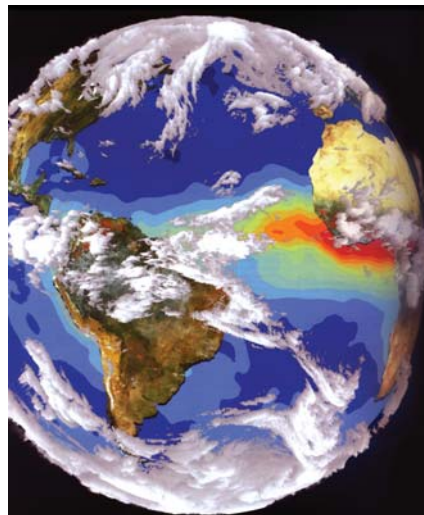


Photo A:

Photo A: Three dimensional model of mycolyltransferase (Rv3804), generated by Modeler. Glu 228, His 260 and Ser 124 correspond to the residues in the catalytic triad.

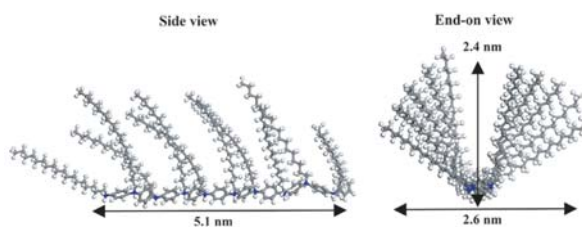


Photo B:

Photo B: Accelrys MS Modeling Program (Materials Studio) was used for visualizing the structure of the oligomeric units of several polymers which were investigated experimentally using the Langmuir-Blodgett ultrathin film technique. A typical example is poly(N-octadecylaniline) was synthesized at the air-water interface, the structure of which is modeled using empirical force field calculations; the geometry optimized decamer unit is shown in the figure above. The computed structure allowed the researchers to interpret features of the ultrathin films revealed by atomic force microscopy.



For more information please contact : **Professor-in-Charge**

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