Centre for Modelling Simulation and Design

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 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 Facility (HPCF) Centre.

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.

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 Modelling, Drug Design and Delivery, Design of new materials, weather forecasting etc. Short term courses have been so far conducted in the areas of Parallel Computing, Monte Carlo Simulation and Molecular Modelling etc.

CMSD has been involved, over the past few years, in promoting and fostering multidisciplinary research programmes in *Advanced Computational Methods*, with focus on the core areas of Physics, Chemistry, Biology, Engineering Sciences and Computer Sciences, besides interest in related research areas like Finite Element Analysis as applied to Nanotechnology, Computational

Fluid Dynamics, Ocean-atmosphere-climate Modelling, High-End-Visualization/Virtual Reality, Modelling and Simulation of large/complex Systems, etc.

Following are the facilities available at the Centre:

1) Data Centre: The Data Centre houses a HPC cluster with following configuration.

A. ***HPC Cluster*****:** 1680 CPU cores, achieving peak 120-Tflops speed, fully networked and consists of the following hardware: HPE Master Nodes(2), Computing Nodes(42), Storage Nodes(2) and SAN storage.

B. ***State of Art Storage Servers:*** Giving High Availability SAN Storage 400TB RAID-5 storage, supports licensed LUSTRE Parallel File System.

C. ***Software:*** Cluster Management Utility (CMU) & Red Hat Enterprise Linux V7.4 (RHEL) OS Software, and GANANA Job Portal Software for job submission with perpetual license and various Open-Source User Application Software such as Gromacs, Python, Gamess, Lammps, R, Absoft Fortran, NAMD, ABINIT, PLUMED, VASP, Molpro,WIEN2k, Desmond etc., have been installed in the HPC. Users can submit and monitor their jobs using a web-based job submission portal GANANA.

2) Seminar Hall:

This is of 80 seat capacity with Wi-Fi internet access, audiovisual equipment, 40 laptops.

3) Two Class Rooms: One with 30 and the other with 17 seats capacity. Each seat in these classrooms are equipped with latest desktops.

Apart from the above, the Centre has one Board Room, two Committee Rooms and a few faculty rooms used for visiting faculty.

Prof. Rajeev Wankar, Professor in School of Computer Sciences is the **Professor-in-Charge of the Centre.**