

Centre for Modelling Simulation and Design

PREAMBLE:

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. 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 center became operational from its new premises in December 2004.

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 and Engineering Science and 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 (HPC) center.

One of the unique academic features of this center 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 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 (DFT), molecular modeling, drug design and delivery, design of new materials etc.

Currently, CMSD has procured the following hardware with assistance of DST-PURSE Phase-II funds:

COMPUTATIONAL FACILITY

HPC Model: HPEDL380, HPEXL170r, HPEDL360, HPEMSA Storage Systems having 40.0 Teraflop Facility.

1. MASTER NODES (2): HPEDL380

HPE ProLiant DL380 Gen10LFF CTO Server with Intel Xeon-G 5115 (10 core, 2.4GHz) processor, 96GB HPE DDR4 Standard Memory (1.5TB maximum), 24 DIMM memory slots, 2x2TB SAS 7.2K SC DS HDD with RAID(1,5,6), HPE 1-Gb Ethernet4-Port 33i Network Adapter, HPE 100Gb 1p OP101 QSFP 28x16 OPA Switch Cluster Interconnect Network, support for NVIDIA GPUs, HPE Insight Cluster Management Utility (CMU),

2. COMPUTE NODES (42): HPEXL170r

Each server node of HPE ProLiant XL170r Gen10 Server can be serviced individually without affecting the operation of other nodes sharing the same chassis to provide increased server uptime. Intel Xeon-G 6148 (2.4GHz, 20C) processor, 192GB/node memory, 2x1TB SATA HDD, HPE 100Gb 1p OP 101 QSFP 28x16 OPA connectivity, HPE Insight Cluster Management Utility (CMU) 8.2. Provides storage and I/O flexibility with drive mapping for enhanced storage allocation.

Total number of cores over all the compute nodes (42) is 1680 (40 cores per node) and the number of threads is 3318; Maximum overall performance of the HPCF is 40 TFlops (0.9524Tflops per node).

3. STORAGE AREA

SAN Storage (1): HPE MSA 1040 (UOH-MSA) HA

400TB RAID-5 storage, supports licensed LUSTRE Parallel File System Ver.2.10.x.

Maximum capacity of the File System: 512PB. Maximum size of a single file (in GB) 31.25PB

Maximum number of files: 4 Billion. Maximum number of files in a directory:

Maximum number of directories: 4x10¹⁰

SAN Storage (1): HPE MSA 2040 (UOH-MSA) PFS

HPE MSA 2040 is a high-performance storage array designed for 8Gb/ 16Gb Fibre Channel, 1GbE/10GbE iSCSI, or 12Gb SAS connectivity with 4 host ports per controller. The MSA 2040 Storage array provides performance balanced support such as consolidation and virtualization.

The MSA 2040 delivers this performance by offering:

- High-performance controller architecture
- 6GB cache per controller, 12GB per storage array
- Support for SSDs, Enterprise SAS HDDs, Midline SAS HDDs, and Self Encrypting Drives
- SAN and SAS interfaces
- Up to four (4) host ports per controller, 8 host ports per storage array
- Two new MSA 2040 Controllers: -
- -MSA 2040 SAN Controller
8Gb/16Gb FC connectivity and/or
1GbE/10GbE iSCSI connectivity
- - MSA 2040 SAS Controller
6Gb/12Gb SAS connectivity

4. STORAGE NODE (2): HPE DL360

HPE ProLiant DL360 Gen10 Server with Intel Xeon-G 5115 (2.4GHz, 10Core) processor, 8GB 2Rx8 PC4-2666V-R Smart Kit, 2x2TB SAS 7.2K LFF SC DS HDD, Smart Array E208i-p SR Gen10 Controller, Gen10 LP Riser Kit, HPE SN1100Q 16Gb 2p FC HBA, 100Gb 1p

OP101 QFSP28x16 OPA Adaptor.

5. SOFTWARE:

The Software comprises Cluster Management Utility (CMU) & Red Hat Enterprise Linux (RHEL) OS Software, and GANANA Job Portal Software (25 users) with perpetual license.

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
 - SLES 10 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 Switches RGB for video & Stereo Audio
- Video and Audio interface — Extron RGB 109
- Audio Amplifier
- NuVision Active Stereo Glasses
- NuVision Stereo Emitters (mid-range)
- Wireless AMX control system
- CEI Ensign Application Software
- Remote Visualization Software Single User

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