

Annual Report 2013-2014

Centre for Modelling, Simulation and Design (CMSD)

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 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 modeling, 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.

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 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 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 a 25.0 Teraflop Facility which is fully networked and consists of the following hardware:

COMPUTATIONAL FACILITY

- 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.
- SGI Altix 4700 a 128 core (Dual Core, Itanium2 9150M 1.67 GHz) shared memory architecture based Unix server comprising of 512 GB RAM
- SGI Altix ICE 8200 EX Cluster [Enhanced] with 1024 core high performance, high throughput and high availability cluster comprising of 1 GB/core memory, built using Infiniband Interconnect.
- SGI XE1300, 2 x Quad core @ 3.0GHz, 4 GB RAM, 146 GB HDDA 128 core Windows CCS/HPC Cluster.
- SGI IS4600 x 2, 100 TBytes of shared Storage system (FC, SATA) for delivering very demanding data intensive environment, leading to High Performance & Productive Computing Facility, through SGI Altix 450 x 2, 8 core, 48 GB RAM, Montvale 1.67 MHz storage servers.
- SGI Spectra T120 Library, 2 x LTO Gen-4 Drives scalable to 6, Spectralogic 100 slots and 60 units of Media, a good tape backup system to archive data with time stamping.
- Management Servers: SGI Altix 250 SERVER x9 (2U), 2 x Quad core, E5472, 3.00 GHz, 1600 FSB, 12MB Cache, 8GB RAM, 6 x 145GB SAS HDD/15K
- Parallel file system to allow bulk I/O operations.
- IBM POWER 7 - 755 Server with - 4 x 8 core 3.3 GHz Power 7 Processor, 2 x 146 GB DASD, 128 GB DDR3 RAM,
- IBM StoreWize V7000 based Storage with 60TB RAW Storage Capacity (30 x 2 TB Disks)
- An integrated linux cluster system with 1.0 TeraFlops computing power having all open source compiler and software for training and executing home grown codes.

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.

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
 - SLES10 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 Switcher RGB for Video & Stereo Audio
- Video and Audio interface – Extron RGB109
- Audio Amplifier
- NuVision Active Stereo Glasses
- NuVision Stereo Emitters (mid range)
- Wireless AMX control system
- CEI Ensign Application Software
- Remote Visualization Software Single User

Visiting Professor

1. Dr. M R Reddy, Metabasis Therapeutics, San Diego, USA.
2. Dr. Inga Ramarao, Computational Physicist, East West Enterprises Inc., USA

Post-Doctoral Fellows

1. Dr (Ms) G. Sai Preeti, recipient of UGC Dr. D. S. Kothari Postdoctoral Fellowship has joined CMSD on February 2011, for a period of 3 years. She previously worked as a Post doctoral research assistant in the Department o di Chimica Fisica ed Inorganica, Università di Bologna, funded by the European Council project 'BIND' after obtaining her PhD from University of Hyderabad.
2. Dr. Jayasri, has been continuing in CMSD as a post-doctoral fellow supported by PURSE. (Dr. Jayasri left CMSD in the month of April-2014)

Invited Talks (Chapter 12)

Prof. V. S. Sastry

1. Invited Talk: "Simulation as a Complementary Tool for Physics Research", at the Refresher Course in Physics, conducted by the Department of Physics, Jawaharlal Nehru Technological University, in August, 2013
2. Invited Talk: "Phase Transitions in Biaxial Nematics: Some Interesting Insights from Monte Carlo Simulations", at the Conference Frontiers in Physics 2013, organized by the School of Physics, University of Hyderabad in September, 2013
3. Invited Talk: "Nuclear Magnetic Relaxometry : Detection of Exclusive Dynamics in Liquid Crystals", at the Andhra Pradesh Science Congress 2013, organized in the University of Hyderabad, in November, 2013
4. Invited Talk: "Application of Nuclear Magnetic Relaxometry to Soft Materials", at the 20th National Conference on Liquid Crystals, held at Manipal University, Manipal, in December, 2013
5. Invited Talk: "Detection of Collective modes in isotropic fluids : Multi-nuclear magnetic relaxation studies", at the Conference on Dynamics of Soft and Biological Materials, in the University of Hyderabad (UoH-TIFRCIS), in January, 2014

Prof. Siba K Udgata

1. Invited Talk "Simulation of soft computing application for high dimensional problem", National workshop on soft computing, Vishakhapatnam, 2014
2. Invited Talk "Sensor network: Theory and applications", International Conference on Frontiers of Intelligent Computing: Theory and Applications (FICTA'2013), Bhubaneswar, 2013

Papers in conferences (chapter 13)

Prof. K.C.James Raju

1. Kumar, G.D.V.S. and Raju, K.C.J., "Whispering gallery modes of planar dielectric resonators in LTCC technology," 2013 Annual International Conference on Emerging

Research Areas and 2013 International Conference on Microelectronics, Communications and Renewable Energy (AICERA/ICMiCR)2013,Vol.1.No.4, pp.1-4, 4-6 June 2013 (PRINT ISBN: 978-1-4673-5150-8), IEEE,DOI: 10.1109/AICERA-ICMiCR.2013.6576026

2. K. Sandeep Sharma, E Srikanth, K.C.James Raju, "Effect of Change in Piezoelectric Layer Thickness in High-Overtone Bulk Acoustic Resonator" Annual International Conference on Emerging Research Areas and 2013 International Conference on Microelectronics, Communications and Renewable Energy (AICERA/ICMiCR)2013,Vol.1,No.4, pp.1-4, 4-6 June 2013 (Print ISBN:978-1-4673-5150-8),IEEE, DOI:10.1109/AICERA-ICMiCR.2013.6576023

3. S.Bashaiah, P.K Sharma, K.C James Raju “High K and Low Loss Dielectrics for High Power Microwave Ceramic Windows” (Oral presentation) has presented at HPRFM-2013 during Sep 4-6, 2013 held at Institute for Plasma Research, Ahmedabad, Gujarat.

4. Bashaiah Sindam, K C James Raju ‘High Permittivity and Low Loss Materials for Reduced Height Waveguide Ceramic Window for High Power Microwave Applications’ (Oral presentation) has presented at IUMRS-2013 during Dec16-20, 2013 held at Indian Institute of Science, Bangalore.

5. Kumar, G.D.V.S. and Raju, K.C.J “ Whispering Gallery Modes of Planar Dielectric Resonators in LTCC Technology”at Annual International Conference on Emerging Research Areas and 2013 International Conference on Microelectronics, Communications and Renewable Energy (AICERA/ICMiCR2013) 4-6 June 2013, at Amal Jyothi Engineering College, Kanjirapally, Kottayam Dt., Kerala, India.

6. K. Sandeep Sharma, E Srikanth, K.C.James Raju, "Effect of Change in Piezoelectric Layer Thickness in High-Overtone Bulk Acoustic Resonator" Annual International Conference on Emerging Research Areas and 2013 International Conference on Microelectronics, Communications and Renewable Energy (AICERA/ICMiCR), 4-6 June 2013, at Amal Jyothi Engineering College, Kanjirapally, Kottayam Dt., Kerala, India.

7. Prasad, K. M. M., Yan, J., Bettiol, A. A., & Raju, K. C J, Microfluidics based Worm Sorter, Comsol Conference, October 17 - 18, 2013.

Prof.V.S.S.Sastry

1. Paper: “Biaxial Liquid Crystal Phases – Insights from Monte Carlo Simulation Studies”, presented by B. Kamala Latha, V.S.S. Sastry and K.P.N. Murthy, in the 20th Conference on Liquid Crystals, held in Manipal University, Manipal, December 16-18, 2013
2. Paper: “Directing Biaxial Transitions in Nematics with an External Field : A Monte Carlo Study”, by Regina Jose, B. Kamala Latha and V.S.S. Sastry, in the 20th on Liquid Crystals, held in Manipal University, Manipal, December 16-18, 2013
3. Paper: “Simulation Study of Biaxial Liquid Crystals Confined in Stripe Patterned Substrates:, by G. Sai Preeti, K.P.N. Murthy and V.S.S. Sastry, in the 20th Crystals, held in Manipal University, Manipal, December 16-18, 2013
4. Paper: “The Effect of Elastic Constants in a Confined Thin Film : Monte Carlo Study”, by Abdul Musavir, G. Sai Preeti and V.S.S. Sastry, in the 20th Crystals, held in Manipal University, Manipal, December 16-18, 2013
5. Paper: “Monte Carlo Study of In-plane Seitching in Confined Liquid Crystal System:, by M. Ramakrishna, G. Sai Preeti and V.S.S. Sastry, in the 20th Crystals, held in Manipal University, Manipal, December 16-18, 2013
6. Paper: “Birefringence, Permittivity, Elasticity, and Rotational Viscosity Measurements in High Birefringent Ambient Temperature Nematic Liquid Crystal Mixtures”, by D. Venkata Sai, P. Satyanarayana, V.S.S. Sastry, P. Kula, R. Dabrowski, and Surajit Dhara, in the 20th National Conference on Liquid Crystals, held in Manipal University, Manipal, December 16-18, 2013

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Prof. Siba K Udgata

1. Energy efficient aggregation in wireless sensor networks for multiple base stations, Reddy Busireddy, N., Udgata, S.K., Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), 8298 LNCS (PART 2), pp. 453-464. (2013)
2. Artificial bee colony algorithm for probabilistic target Q-coverage in wireless sensor networks, Mini, S., Udgata, S.K., Sabat, S.L., Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), 8297 LNCS (PART 1), pp. 446-456 (2013).
3. A Secure and Reliable Mobile Banking Framework, Ahamad, S.S., Sastry, V.N., Udgata, S.K., Nair, M. Advances in Intelligent Systems and Computing, 249 VOLUME II, pp. 741-748. (2014)

4. A Secure Lightweight and Scalable Mobile Payment Framework, Ahamad, S.S., Udgata, S.K., Nair, M., *Advances in Intelligent Systems and Computing*, 247, pp. 545-553. (2014)

Refereed Journal Publications (Chapter 14)

Prof. K.C.James Raju

1. Bashaiah Sindam, Pramod K.Sharma and K.C.James Raju “Design and analysis of stepped impedance transformer from air filled waveguide to dielectric filled waveguide for high power microwave window applications” *Mater. Res. Express*, 1, 015701, 2014.

V.S.S. Sastry

1. Lattice spin simulations of topological defects in biaxial nematic films with homeotropic surface alignment, G. Sai Preeti, C. Zannoni, C. Chiccoli, P. Pasini, and V.S.S. Sastry, *Int. J. Mod. Phys. C*, 24, 1350026 (2013)
2. Birefringence, permittivity, elasticity and rotational viscosity of ambient temperature, high birefringent nematic liquid crystal mixtures, D. Venkata Sai, P. Sathyanarayana, V.S.S. Sastry, J. Heman, P.Kula, R. Dabrowski, and S. Dhara, *Liq. Cryst.*, 41, 591 (2014)
3. Detection of an intermediate biaxial phase in the phase diagram of biaxial liquid crystals : Entropic sampling study, B. Kamala Latha, Regina Jose, K.P.N. Murthy and V.S.S. Sastry, *Phys. Rev. E (Rapid Comm.)*, 89, 050501 (2014)

Prof. K. Senthilkumar

1. Theoretical investigation of interaction between Psoralen and Alzetamine with stacked DNA base pairs. P.Deepa, P.Kolandaivel and K.Senthilkumar *Mat.Sci.Eng.C.*, (2012), 32, 423-431.
2. Coordination and binding properties of zwitterionic metal cations glutathione with transition metal cations. R.Shankar, P.Koladaivel, L.Senthil Kumar *Inorg.Chim.Acta.*, (2012), 387, 125-136
3. Structural Properties and the effect of platinum drugs with DNA base pairs.P.Deepa, P.Koladaivel, K.Senthilkumar *Struct.Chem.*, (2013) 24, 583-595

4. Study of mutation and misfolding of Cu-Zn SOD1 Protein. S.P.Keerthana & P.Kolandaivel *J.Biomol.Struct.Dyn.*, (2013), DOI:10.1080/07391102.2013.865104.
5. Study on the disulfide bond and disulfide loop of native and mutated SOD1 protein. S.P.Keerthana, P.Kolandaivel *J.Mol.graph.Model.*, (2014), 50, 78-89.

Vaitheeswaran, G

1. Electronic structure and optical properties of $\text{Ca}(\text{NH}_2\text{BH}_3)_2$ studied from GW calculations Bheema Lingam,C., Ramesh Babu,K., Tewari, S.P., Vaitheeswaran, G. , Lebègue, S.*Journal of Physical Chemistry C* 115 (38) , pp. 18795-18801(2011)
2. Thermoelastic properties of ScB_2 , TiB_2 , YB_4 and HoB_4 : Experimental and theoretical studies Waśkowska, A., Gerward, L. , Staun Olsen, J., Ramesh Babu, K., Vaitheeswaran, G., Kanchana, V., Svane, A., Filipov, V.B., Levchenko, G., Lyaschenko, A,*Acta Materialia* 59 (12) , pp. 4886-4894(2011)
3. Structural, electronic, bonding, and elastic properties of NH_3BH_3 : A density functional study Bheema Lingam,C., Ramesh Babu, K., Tewari, S.P.ab, Vaitheeswaran, G, *Journal of Computational Chemistry* 32 (8) , pp. 1734-1742 (2011)
4. High-pressure study of lithium azide from density-functional calculations Ramesh Babu, K., Bheema Lingam, C., Tewari, S.P., Vaitheeswaran, G.,*Journal of Physical Chemistry A* 115 (17) , pp. 4521-4529(2011)
5. Electronic structure, optical properties, and bonding in alkaline-earth halofluoride scintillators: BaClF , BaBrF , and BaIF Yedukondalu, N., Ramesh Babu, K., Bheemalingam, C., Singh, D.J., Vaitheeswaran, G., Kanchana, V.,*Physical Review B - Condensed Matter and Materials Physics* 83 (16) , art. no. 165117(2011)
6. Structural, thermodynamic and optical properties of MgF_2 studied from first-principles theory Ramesh Babu, K., Bheema Lingam, C., Auluck, S., Tewari, S.P., Vaitheeswaran, G.,*Journal of Solid State Chemistry* 184 (2) , pp. 343-350(2011)
7. Quantum chemical studies on beryllium hydride oligomers Bheema Lingam,C, Ramesh Babu, K., Tewari, S.P., Vaitheeswaran, G.,*Computational and Theoretical Chemistry* 963 (2-3) , pp. 371-377(2011)

8. Quasiparticle band structure and optical properties of NH_3BH_3 Bheema Lingam, C., Ramesh Babu, K., Tewari, S.P., Vaitheeswaran, G., Lebègue, S., *Physica Status Solidi - Rapid Research Letters* 5 (1) , pp. 10-12(2011)
9. Metal azides under pressure: An emerging class of high energy density materials Vaitheeswaran, G., Ramesh Babu, K., *Journal of Chemical Sciences* 124 (6) , pp. 1391-1398(2012)
10. Vibrational properties of BaClF , BaBrF and BaIF under high pressure Yedukondalu, N., Vaitheeswaran, G. *Journal of Physics: Conference Series* 377 (1) , art. no. 012070(2012)
11. High pressure study on structural and vibrational properties of NH_3BH_3 Bheema Lingam, C., Ramesh Babu, K., Tewari, S.P., Vaitheeswaran, G., *Journal of Physics: Conference Series* 377 (1) , art. no. 012088(2012)
12. Computational study of structural, electronic, and optical properties of crystalline NH_4N_3 Yedukondalu, N., Ghule, V.D., Vaitheeswaran, G. *Journal of Physical Chemistry C* 116 (32) , pp. 16910-16917(2012)
13. Effect of van der Waals interactions on the structural and elastic properties of black phosphorus Appalakondaiah, S., Vaitheeswaran, G., Lebègue, S., Christensen, N.E., Svane, A., *Physical Review B - Condensed Matter and Materials Physics* 86 (3) , art. no. 035105(2012)
14. Ab-initio study of structural and vibrational properties of KN_3 under pressure Ramesh Babu, K., Vaitheeswaran, G., *Chemical Physics Letters* 533 , pp. 35-39(2012)
15. Density functional study of electronic, bonding, and vibrational properties of $\text{Ca}(\text{NH}_2\text{BH}_3)_2$ Bheema Lingam, C, Ramesh Babu, K., Tewari, S.P., Vaitheeswaran, G., *Journal of Computational Chemistry* 33 (9) , pp. 987-997(2012)
16. Structural properties of solid nitromethane: A density functional study Appalakondaiah, S., Vaitheeswaran, G., *AIP Conference Proceedings* 1512 , pp. 830-831
17. Ab initio study of electronic structure, elastic and optical properties of anti-perovskite type alkali metal oxyhalides Ramanna, J., Yedukondalu, N., Ramesh Babu, K., Vaitheeswaran, G., *Solid State Sciences* 20 , pp. 120-126(2013)

18. Pressure induced structural phase transition in solid oxidizer KClO_3 : A first-principles study Yedukondalu, N., Ghule, V.D., Vaitheeswaran, G. *Journal of Chemical Physics* 138 (17), art. no. 174701(2013)
19. A DFT study on structural, vibrational properties, and quasiparticle band structure of solid nitromethane Appalakondaiah, S., Vaitheeswaran, G., Lebègue, S., *Journal of Chemical Physics* 138 (18), art. no. 184705(2013)
20. Structure, elastic and dynamical properties of KN_3 and RbN_3 : A van der Waals density functional study Ramesh Babu, K., Vaitheeswaran, G., *Solid State Sciences* 23, pp. 17-25(2013)
21. Structural, elastic, electronic and optical properties of layered alkaline-earth halofluoride scintillators Kanchana, V., Yedukondalu, N., Vaitheeswaran, G. *Philosophical Magazine* Vol. 93, No. 26, 3563–3575(2013)
22. Lattice dynamics and electronic structure of energetic solids LiN_3 and NaN_3 : A first principles study Ramesh Babu, K., Vaitheeswaran, G. *Chemical Physics Letters* 586, pp. 44-50 (2013).
23. High-Pressure Structural Stability and Optical Properties of Scheelite-type ZrGeO_4 and HfGeO_4 X-ray Phosphor Hosts G. Shwetha, V. Kanchana, K. Ramesh Babu, G. Vaitheeswaran, M. C. Valsakumar, *J. Phys. Chem. C* 2014, 118, 4325–4333
24. Structural, vibrational, and quasiparticle band structure of 1,1-diamino-2,2-dinitroethelene from ab initio calculations Appalakondaiah, S., Vaitheeswaran, G., Lebègue, S., *Volume 140, Issue 1, 2014, Article number 014105.*
25. Structural and vibrational properties of nitrogen-rich energetic material guanidinium 2-methyl-5-nitraminotetrazolate Ramesh Babu, K., Vaitheeswaran, G., *Chemical Physics Letters* Volume 592, 30 January 2014, Pages 132-137.
26. Thermoelectric properties of marcasite and pyrite FeX_2 (X = Se, Te): A first principle study Gudelli, V.K., Kanchana, V., Vaitheeswaran, G., Valsakumar, M.C., Mahanti, S.D., *RSC Advances* Volume 4, Issue 19, 2014, Pages 9424-9431
27. Structural, electronic and optical properties of novel carbonate fluorides $\text{ABC}_3\text{O}_3\text{F}$ (A=K, Rb, Cs; B=Ca, Sr) Narsimha Rao, E., Appalakondaiah, S., Yedukondalu, N., Vaitheeswaran, G. *Journal of Solid State Chemistry* Volume 212, April 2014, Pages 171-179

28. Structural properties of solid energetic materials: A van der Waals density functional study Vaitheeswaran, G., Ramesh Babu, K., Yedukondalu, N., Appalakondaiah, S. Current Science, Volume 106, Issue 9, May 2014, Pages 1219-1223

29. Polymorphism and thermodynamic ground state of silver fulminate studied from van der Waals density functional calculations N. Yedukondalu and G. Vaitheeswaran Journal of Chemical Physics 140, 224705 (2014)

30. Structural, elastic, optical properties and quasiparticle band structure of solid cyanuric triazide Appalakondaiah, S., G. Vaitheeswaran, Lebègue, S. Chemical Physics Letters Volume 605-606, Pages 10-15 (2014).

31. Density functional study of electronic structure, elastic and optical properties of MNH₂ (M=Li, Na, K, Rb) Ramesh Babu, K., and Vaitheeswaran, G., 2014 J. Phys.: Condens. Matter 26, 235503 (2014).

Prof. Siba K Udgata

1. Sensor deployment and scheduling for target coverage problem in wireless sensor networks, Mini, S., Udgata, S.K., Sabat, S.L. IEEE Sensors Journal, 14 (3), art. no. 6637016, pp. 636-644. (2014)
2. A Secure and Optimized Proximity Mobile Payment Framework with Formal Verification, SS Ahamad, VN Sastry, SK Udgata, International Journal of E-Services and Mobile Applications (IJESMA) Vol. 6, 2014
3. A Secure Mobile Payment Framework in MANET Environment, SS Ahamad, VN Sastry, SK Udgata, International Journal of E-Business Research (IJEER) 9 (1), 54-84 (2013)
4. Secure mobile payment framework based on uicc with formal verification, Ahamad, S.S., Sastry, V.N., Udgata, S.K. International Journal of Computational Science and Engineering, 9 (4), pp. 355-370. (2014)
5. Field programmable gate arrays-based differential evolution coprocessor: A case study of spectrum allocation in cognitive radio network, Anumandla, K.K., Peesapati, R., Sabat, S.L., Udgata, S.K., Abraham, A. (2013) IET Computers and Digital Techniques, 7 (5), pp. 221-234. (2013)

Ongoing project(s) - Chapter 15:

1. "Development of wireless sensor network based adaptive water quality and quantity monitoring system (AquaSense)" sponsored by Information Technology Research Academy (ITRA), Department of Electronic and Information Technology (DeITy), Govt. of India. It is a multi-institutional project headed by CMSD, University of Hyderabad (PI: Prof. Siba K Udgata)

2. “Noise Modelling and Sensitivity Analysis of Fibre Optics based Accelerometer based Sensor” sponsored by Research Center Imarat (RCI), DRDO, Hyderabad.
3. DST sponsored project on *Computer Simulations and NMR Investigations of Responsive Materials for Photonics Applications*, under Indo-Italian Joint Collaboration scheme, with Professor Claudio Zannoni of the University of Bologna, Bologna, Italy, from June 2012 for three years:

Seminars and Workshops conducted:

1. Department of Biotechnology Conducted a Workshop on Programming on R and Applications in Computational Biology during January 10-13, 2013 at CMSD, University of Hyderabad.
2. Centre for Neural & Cognitive Sciences is Conducted Indo-Italian Training Workshop on EEG & MEG DATA PROCESING during April 1-4, 2013 at CMSD, University of Hyderabad.
3. CMSD and C-DAC, Pune University Campus are Jointly Conducted a Workshop on Hybrid Computing - Co-Processors / Accelerators-Power-aware Computing - Performance of Application Kernels during October 15-18, 2013 at CMSD, University of Hyderabad.
4. CRRAO-AIMSCS (C R Rao Advanced Institute of Mathematics, Statistics and Computer Science, UoH), CMSD and CSI are jointly conducted National Workhsop on Big Data Analytics (BIDA-2014) during August 22-24, 2014 BIDA-2014 (National Workhsop on Big Data Analytics)

Prof. Siba K Udgata is the Professor-in-Charge of the CMSD. Prof. V S S Sastry is Resource Coordinator and Prof. K P N Murthy is Academic Coordinator.