

Center of Excellence

Advanced Computational Research and
Education

(MHRD /CC /20130176)

Currently Coordinated by

Dr. Yatindra Nath Singh

Head, Computer Center and Associate Dean
Digital Infrastructure

Indian Institute of Technology Kanpur
Uttar Pradesh

Objective

- Provisioning of Computation Infrastructure
- Use by Doctoral Students and Faculty for computational research in various domains

Publications in last six months

- Halder, P., Maurya, M., Jain, S.K., Singh, J.K. Understanding adsorption of CO₂, N₂, CH₄ and their mixtures in functionalized carbon nanopipe arrays (2016) Physical Chemistry Chemical Physics, 18 (20), pp. 14007-14016.
- Bhateja, A., Sharma, I., Singh, J.K. Scaling of granular temperature in vibro-fluidized grains (2016) Physics of Fluids, 28 (4), art. no. 043301,.

- Katiyar, P., Patra, T.K., Singh, J.K., Sarkar, D., Pramanik, A. Understanding adsorption behavior of silica nanoparticles over a cellulose surface in an aqueous medium (2016) *Chemical Engineering Science*, 141, pp. 293-303.
- Kommu, A., Namsani, S., Singh, J.K. Removal of heavy metal ions using functionalized graphene membranes: A molecular dynamics study (2016) *RSC Advances*, 6 (68), pp. 63190-63199.

- Namsani, S., Singh, J.K. Dewetting dynamics of a gold film on graphene: Implications for nanoparticle formation(2016) Faraday Discussions, 186, pp. 153-170.
- Bhandary, D., Benková, Z., Cordeiro, M.N.D.S., Singh, J.K. Molecular dynamics study of wetting behavior of grafted thermo-responsive PNIPAAm brushes (2016) Soft Matter, 12 (12), pp. 3093-3102.

- Investigation of the Sensitivity of Turbulent Closures and Coupling of Hybrid RANS-LES Models for Predicting Flow Fields With Separation and Reattachment
Author name: G. Kumar, S. K. Lakshmanan, H. Gopalan and A. De
Journal: INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS
DOP: Sep, 2016 (DOI: 10.1002/flid.4334)
- Stabilization of lifted hydrogen jet diffusion flame in a vitiated coflow: effects of jet and coflow velocities, coflow temperature and mixing. **Santanu De**, Ashoke De, Abhishek Jaiswal, Arpita Dash, Int. J. Hydrogen Energy, 41(33), 15026 – 15042, 2016.

- Quantification of Aromaticity Based on Interaction Coordinates: A New Proposal, Sarvesh Kumar Pandey, Dhivya Manogaran, Sadasivam Manogaran and Henry F. SchaeferIII, J. Phys. Chem. A, 2016, 120, 2894-2901.
- Manjusha Chugh and Madhav Ranganathan, J. Phys. Chem. C, 2016, 120, 8076
- A. Pandey and M. K. Verma, *Scaling of large-scale quantities in Rayleigh-Bénard convection*, Phys. Fluids **28**, 095105 (2016)

- Paramita Ghosh and Madhav Ranganathan, J. Cryst. Growth, in press. DOI: <http://dx.doi.org/10.1016/j.jcrysgro.2016.03.015>
- R. N. V. Krishna Deepak and R. Sankararamakrishnan. Unconventional N-H...N hydrogen bonds involving proline backbone nitrogen in protein structures. Biophysical Journal 110, 1967-1979 (2016)
- A. Pandey, M. K. Verma, A. G. Chatterjee, and B. Dutta, *Similarities between 2D and 3D convection for large Prandtl number*, Pramana – J. Phys. **87**, 13 (2016)

- R. N. V. Krishna Deepak and R. Sankararamakrishnan. N-H...N hydrogen bonds involving histidine imidazole nitrogen atoms: A new structural role for histidine residues in proteins. *Biochemistry* 55, 3774-3783 (2016)
- Ambrish Pandey, *Scaling of large-scale quantities in Rayleigh-Bénard convection*, Thesis submitted to the Department of Physics, IIT Kanpur in May 2016.
- Abhishek Kumar, *Energy spectra and fluxes of buoyancy-driven turbulent flows*, Thesis submitted to the Department of Physics, IIT Kanpur in September 2016

- A. Pandey, A. Kumar, A. G. Chatterjee, and M. K. Verma, *Dynamics of large-scale quantities in Rayleigh- Bénard convection*, Submitted to Phys. Rev. E (2016)
- D. Nath, A. Pandey, A. Kumar, and M. K. Verma, *Near isotropic behavior of turbulent thermal convection*, Submitted to Phys. Rev. Fluids (2016)
- Velachi, V., Bhandary, D., Singh, J.K., Cordeiro, M.N.D.S. Striped gold nanoparticles: New insights from molecular dynamics simulations (2016) Journal of Chemical Physics, 144 (24), art. no. 244710

- The Wacker Oxidation of Allyl Alcohol along Cyclic-Intermediate Routes: an Ab Initio Molecular Dynamics Investigation, Venkataramana Imandi and Nisanth N. Nair, Chem. Phys. Lett. 660, 111-116 (2016).
- Insights into the Mechanism and Kinetics of Thermo-Oxidative Degradation of HFPE High Performance Polymer, Sooraj Kunnikuruvan, Priya V. Parandekar, Om Prakash, Tom K. Tsotsis, and Nisanth N. Nair, J. Phys. Chem. B. 120, 4852-4860 (2016).
- CPMD/GULP QM/MM Interface for Modeling Periodic Solids: Implementation and its Application in the Study of Y-Zeolite Supported Rh_n Clusters, Sudhir K. Sahoo and Nisanth N. Nair, J. Comput. Chem. 37, 1657-1667 (2016).

- Deacylation Mechanism and Kinetics of Acyl-Enzyme Complex of Class-C β -Lactamase and Cephalothin, Ravi Tripathi, and Nisanth N. Nair J. Phys. Chem. B 120, 2681-2690 (2016).
- Sampling Free Energy Surfaces as Slices by Combining Umbrella Sampling and Metadynamics, Shalini Awasthi, Venkat Kapil and Nisanth N. Nair, J. Comput. Chem. 37, 1413-1424 (2016)

Research Students involved in the Center

- Dr. Tarak K. Patra, 2008
- Ambrish Pandey (2010)
- Dr. Chandan Das, 2009
- Dr. Ashish Bhateja, 2009
- RAHUL KUMAR SONI (2012)
- Dr. Debdip Bhandary, 2010
- Sanjeev Kumar Ghai (2014) – PhD scholar
- Namsani Sadanandam, 2011
- ALOK MISHRA (2013)

- Anitha Kommu, 2011
- Mukesh Adlak (2015) – M.S. by Research
- Atanu K. Metya, 2012
- PRADEEP KUMAR S (2013)
- Parul Katiyar, 2013
- NITISH ARYA (2015)
- Manish Maurya, 2013
- GAURAV KUMAR (2016)
- Sarvesh Kumar Pandey
- Soumyadeb Dey

- R. N. V. Krishna Deepak (Thesis submitted)
- Manu Vajpai (Dec. 2010)
- Mishtu Mukherjee (July 2011)
- C. Narendra Reddy (Dec. 2012)
- Abhishek Kumar (2011)
- Ankita Gupta (July 2014)
- Rahul Verma, July 2016
- Anando G. Chatterjee (2012)

Fund situation

- Sanctioned amount: 5,70,00,000
- Released amount so far: 1,05,00,000
- Current balance: (-) 41,19,886

Next six month requirement

Deliverables	Likely cost (in Rs.lakhs)
PBS Portal, Scheduler, Compute Manager AMC	30
AMC of HPC 2010 extension	35
AMC of HPC 2010	100
Software Upgrade and AMC	30
UPS AMC etc.	5
Additional HPC Servers AMC	5
Training	10
Research Expenses	20
Research related Travel	10
Total	245
Balance	(-)41.19886
Funds needed	286.19886