

# **Usage of SERC SahasraT Supercomputer for Scientific Applications in IISc in 2017**



**Supercomputer Education and Research Centre**

**Indian Institute of Science**

**Bangalore – 560012**

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# SERC Cray SahasraT System

SERC is home to one of the fastest super computers in India, the Cray XC40, known as SahasraT in IISc. It is a system that combines the capabilities of Intel's latest Xeon Haswell processors for the CPU cluster and Nvidia's K40 series of GPU cards and Intel's Xeon-Phi 7210 cards for the accelerator cluster connected using Cray's own Aries high-speed interconnect on a dragonfly topology with DDN's high performance storage units.

It is a 1.4 PFlop system with 33000 Intel Haswell cores with total memory of 176 TB RAM, and 2 PB of storage. It also has accelerator clusters each with 44 nodes of one NVIDIA K40 GPU card, and 24 nodes each with one Intel Xeon Phi card.

System also hosts architecture specific parallel libraries like OpenMP, MPI, CUDA and Intel Cluster software. Extensive range of parallel Scientific and Mathematical libraries like BLAS, LAPACK, Scalapack, fftw, hdf5, netcdf, PETSc, Trilinos etc. are also available on the system.

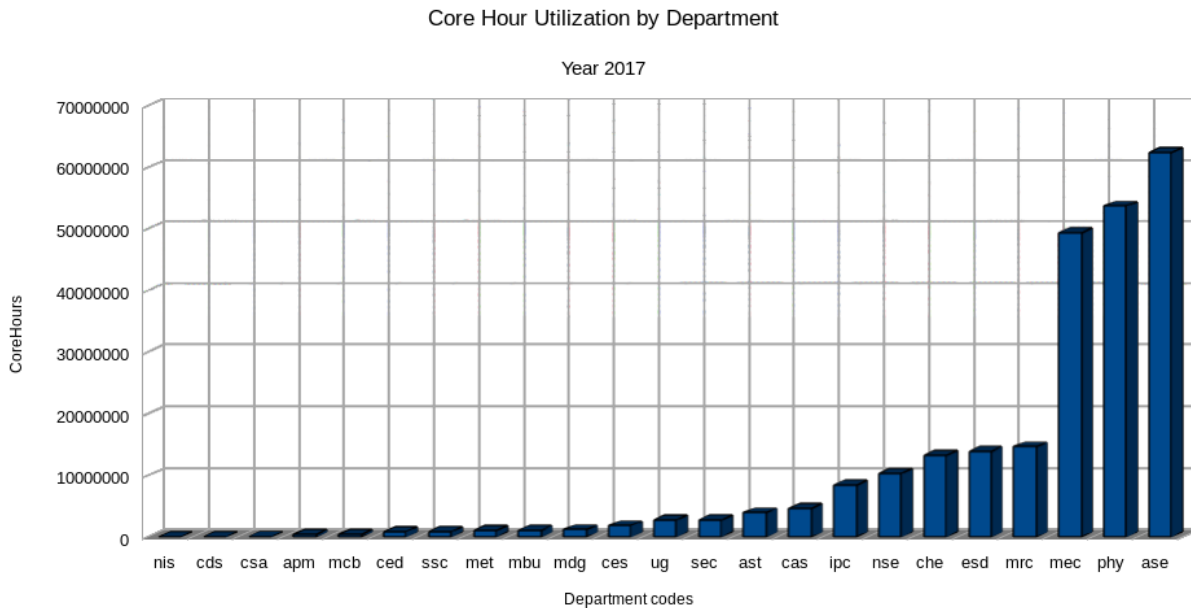
The CRAY XC40 facility uses PBS (Portable Batch System) to schedule jobs. The scheduler for batch jobs in SahasraT uses the FCFS (First-Come, First-Served), based on queue priority and backfilling techniques to achieve the highest system utilization possible with a reasonable turn-around time.

There are eight queues configured on the Cray XC40 with limitations on job size in terms of cores requested, wall time and number of jobs on queue and in the running state. Large and medium jobs are prioritized, over small jobs.

## Usage in 2017

SahasraT serves 24 Departments, 76 Research Labs and over 215 users. Following are some salient statistics of the usage of SahasraT in 2017.

- SahasraT processed a total 94000 jobs in 2017, i.e. an average of about 7800 jobs per month.
- The total system utilization is about 250 million core hours, i.e., an average system utilization of about 20 million core hours per month
- The usage by the different departments in 2017 is given by the following chart:



## IISc's Scientific Applications on SahasraT

In 2017, a large number of scientific applications were executed by the Institute community on SahasraT. These belonged to different departments including Aerospace, Physics, Centre for Atmospheric and Oceanic Sciences (CAOS), Materials Research Centre (MRC), Chemistry and Mechanical Engineering. The applications spanned different domains including study of turbulence, climate modeling, computational fluid dynamics, large eddy simulations, flow of granular materials, design of novel topological materials, hydrodynamics, study of galaxy clusters, DNA nanotechnology, protein synthesis, study of glass properties, crystallography etc.

The following sections gives details of the usage of SahasraT for various computational science problems.

# Aerospace

## Prof. N Balakrishnan's Lab

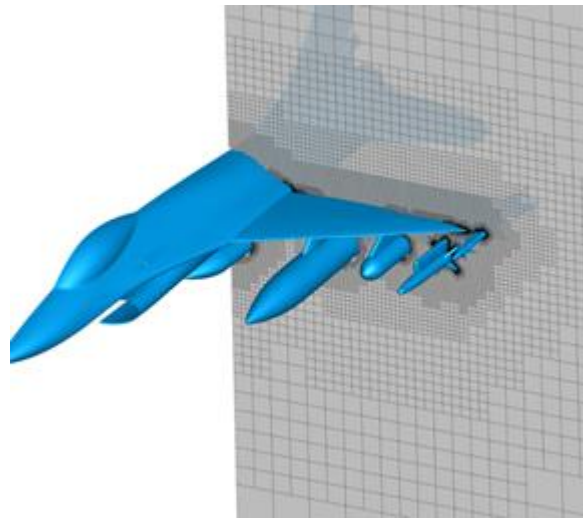
**Team:** Computational aerodynamics

**Research Areas** (Details below): (1) Unsteady aerodynamics: Dynamic ground effect, Scramjet intake flows (2) Optimization (3) Meshless solvers: Cartesian mesh calculations (4) High lift Aerodynamics

**SahasraT Usage:** 1.7 million core hours.

**Experimental Setup:** MPI Parallel HiFUN solver is used.

**Performance:** In the Computational Aerodynamics lab, we have an heterogenous platform with about 700 Xeon cores. Typically, 250 or 500 of these cores are allocated for a given job. On the other hand, our usage of the Cray system ranges from 1000 cores to over 10000 cores, depending upon the nature of the problem (steady/unsteady etc.) and the availability of the queue. Typically, in a 24 hr queue, several steady simulations and one unsteady simulation can be accomplished with 10000 cores. It should be noted that the unsteady simulations cannot be accomplished with the kind of resource we have in the lab. In the next few months, we also intend to start unsteady simulations of higher fidelity, which would typically require several days usage of about 10000 cores.



**Figure:** Cartesian point distribution around a combat aircraft for the LSFD-U Solver

### Publications

1. Mohamed Yousuf, N. Balakrishnan, *Residual based mesh adaptation for Meshless LSFD-U solver*, AIAA 2017-3104.

2. Mondal, Partha and Kanale, Anup V and Balakrishnan, N and Shende, Nikhil V and Wadnerkar, Rohan Pradeep (2017), *Optimization of Flap Position Using a Modified Discrete-Vortex Method*, AIAA Journal, Vol. 55 (12). pp. 4083-4093.

## Prof. Joseph Matthew's Lab

**Team:** Laboratory for turbulence computations

**Research Areas** (Details below): Large eddy simulations, study of canonical flows

**SahasraT Usage:** 33.7 million core hours.

**Experimental Setup:** The codes were parallelized using MPI. 1000+ cores on Cray XC40 were used for the simulations.

**Problem Size Scaling:** The Cray system allowed exploration of large-size systems involving at least  $(10^6)$  grid points.

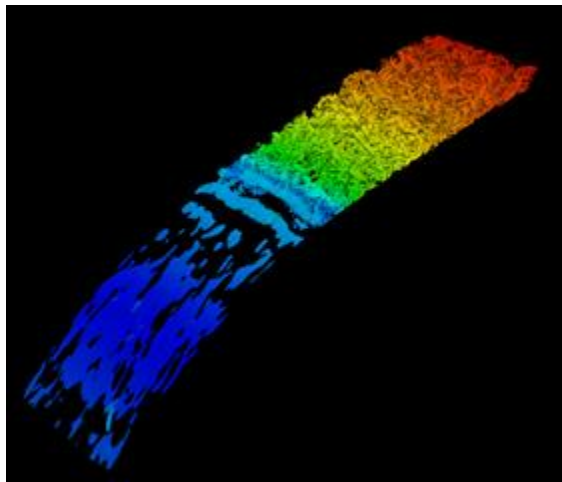
### Details of Research

#### Large Eddy Simulations

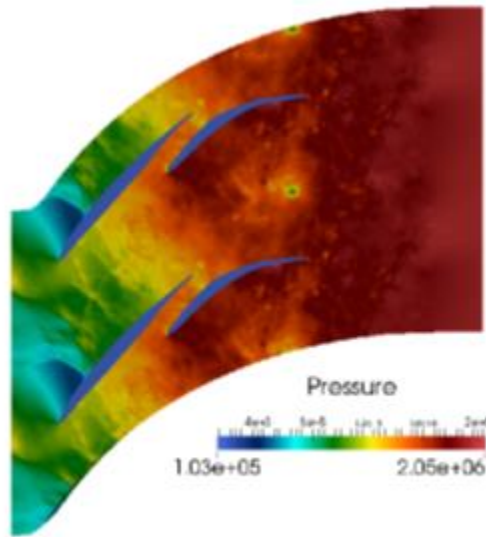
This study involves large eddy simulations (LES) of flow in turbomachine blade passages. These are problems with 10--20 million gridpoints. Sometimes these solutions, which present unexpected features, are verified using direct numerical simulations with about 100 million points. These types of simulations are also carried out for high-speed, sometimes supersonic jets. While these are closer to applications, the studies are to establish the correctness of the methods for wider classes of flows. A newer study is of LES for combustion.

#### Study of Canonical Flows

A second type of study is of instabilities in canonical flows like the breakdown of a jet, and vortex breakdown.



*Figure: The 2D view is from a large computation with supersonic flow: dark blue to cyan is a strong shock.*



*Figure: The 3D view uses  $O(10^6)$  grid points (5 basic fields, but probably at least 10 more)*

### **Publications**

1. Mitra, P., Kantharaju, J., Rayan, R., & Mathew, J. (2017). Large Eddy Simulation of Tandem Blade Stator Cascades. In ASME Turbo Expo 2017: Turbomachinery Technical Conference and Exposition. doi:10.1115/GT2017-64286
2. Mondal, P. & Mathew, J. (2017). Large eddy simulation of a compressor stage. In ASME 2017 Gas Turbine India Conference. Paper GTIndia 2017-4849.
3. Rizvi, S. A. H., & Mathew, J. (2017). Large Eddy Simulation of Transitional Flow in a Compressor Cascade. In ASME Turbo Expo 2017: Turbomachinery Technical Conference and Exposition. doi:10.1115/GT2017-64279.

## **Prof. ON Ramesh's Lab**

**Research Areas** (Details below): Numerical simulations of turbulent flows

**SahasraT Usage:** 3.65 million core hours

**Experimental Setup:** The codes were parallelized using MPI. 264 cores on Cray XC40 were used for the simulations.

**Performance:** A single run usually takes about two weeks on Cray machine with 264 cores.

### **Details of Research**

#### **Numerical simulations of turbulent flows**

We are working on numerical simulations of turbulent flows. With the help of supercomputers, it is possible to solve a set of non-linear partial differential equations that govern fluid flow. Solving turbulence problem is especially complex and computationally intensive. The simulations generate very useful data which can be used for a wide range of applications in aerospace industry as well as for fundamental research in turbulence.

## **Prof. Santosh Hemchandra's Lab**

**Research Areas** (Details below): Gas-turbine combustor flow, noise radiation from multiple interacting jets and turbulent reacting flows

**SahasraT Usage:** 16.8 million core hours

**Experimental Setup:** The primary resource used by our Lab is the CRAY XC40 which has enabled us to simulate experiments that were hitherto out of reach due to the limitation on scaling imposed by the older pre-existing clusters in AE as well as in SERC. Typically our jobs used 1000 – 4000 cores. Based on 2017 experience, we plan to scale up to 8000 cores and beyond in 2018.

All MPI based I/O is performed using non-blocking asynchronous calls in order to overlap computation and communication and mitigate the latency introduced by the former. Broadcast communication is performed only once during setup of data structures. All communication is point-to-point thereafter during time stepping ensuring we keep bandwidth usage to a minimum. File I/O is performed using HDF5 parallel I/O routines as per the recommendations on the HDF5 Lab website.

**Performance:** Most of the cases we run are not possible to execute on our external systems as they would not fit within memory. Some of the smaller cases we've run on the small queue and used for scaling tests on the medium queue have shown linear scaling upto 9600 cores.

## Details of Research

### Gas-turbine combustor flow, Noise Radiation from Multiple Interacting Jets, Turbulent Reacting Flows

Our Lab's work in 2017 involved in performing time accurate LES simulations of multi-element swirl flows of relevance to improve our fundamental understanding of unsteady behavior of Gas-turbine combustor flow, noise radiation from multiple interacting jets and turbulent reacting flows. The algorithm discretizes the fully compressible reacting Navier-Stokes equations on a structured multiblock CFD mesh using a finite difference approach. Time integration is achieved using a Runge-Kutta method. The solver we use is a multiblock structured CFD solver with support for overset meshes which allows for ease of meshing complex flow geometries. ANSYS-ICEM CFD procured independently in the department is being used for Meshing. The solver can import meshes in CGNS format as well as a native HDF5 based format defined by our Lab.

### Publications

1. Nishanth Muthichur, Santosh Hemchandra and Arnab Samanta, "Aeroacoustic noise sources in Mach 0.9 interacting twin jets", submitted to AIAA Aviation meeting, June 2018 (acceptance awaited).

## Prof. Swetaprovo Chaudhuri's Lab

**Team:** Turbulent Reacting Flow Physics . S. Chaudhuri, H. Dave, A. Kalbhor, A. Moitra, A. Mohan.

**Research Areas** (Details below): Turbulent reacting flow physics.

**SahasraT Usage:** 1.8 million core hours

**Performance:** The various resources used during our work are Cray XC40, Tyrone cluster, and Dell visualization server. The number of cores used during each project are listed below-

On-the-fly flame particle tracking- 960 processors

Lagrangian flame-element analysis- 1008 processors

Flame speed response to stretch rates- 480 processors

Auto-ignition study- 96 processors

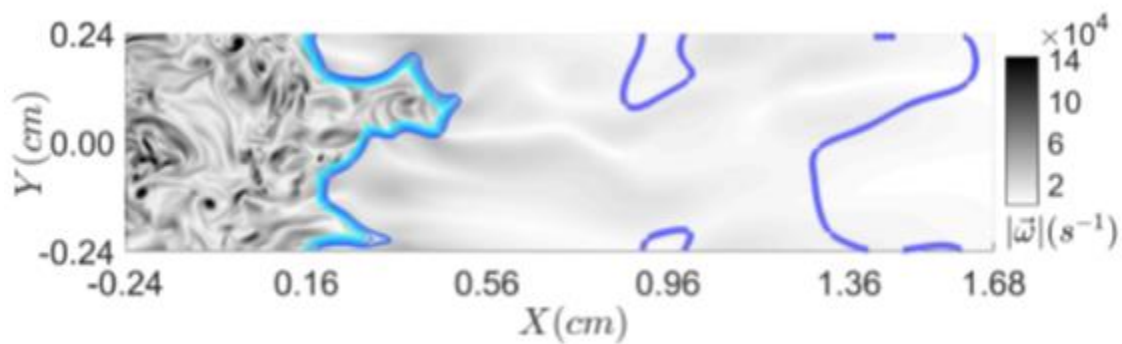
Turbulence facilitated ignition- 720 processors

**Experimental Setup:** Typical execution time for one simulation in HPC systems was about 72 hrs. The systems in our lab are single processor systems, therefore running large simulations in the systems is not feasible, and a direct comparison of runtime cannot be made. However, the typical execution time of the systems is around 87 microseconds per time step per meshpoint versus 0.865 microseconds per time step per meshpoint achieved using just 24 processors in the HPC system. The projects made use of a finite difference open source code, called the pencil code, which is parallelized using MPI.

## Details of Research

### Turbulent Reacting Flow Physics

A number of projects were carried out during the past year in the Turbulent Reacting Flow Physics using **SERC's** HPC systems. We studied turbulent reacting flows with the help of Direct Numerical Simulations (DNS). A two dimensional slice of a typical computational domain along with a turbulent flame front is shown in figure 1.

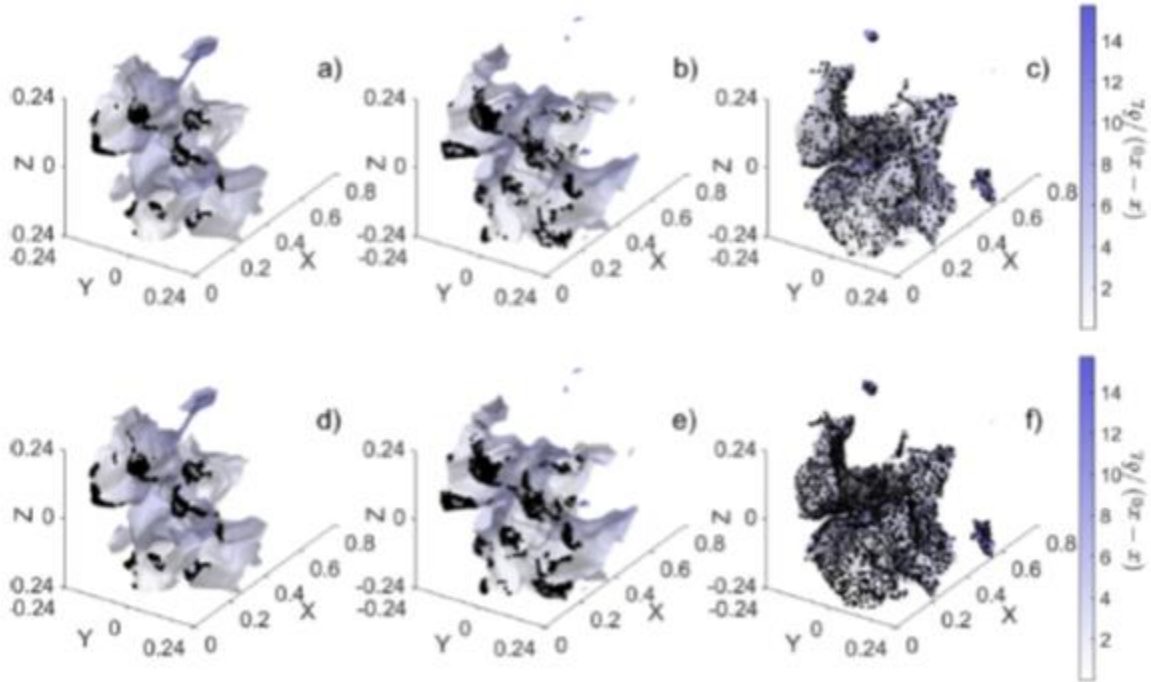


*Figure 1: Computational domain showing turbulence-chemistry interaction. The figure shows the wrinkled flame front and vertices in a turbulent mixture of hydrogen and air.*

Following is a list of the projects undertaken and their applications:

- A new method called on-the-fly flame particle tracking for tracking tracer particles on a turbulent flame front, solving their evolution within the DNS solver, was developed and used for studying the mechanics of flame annihilation (by analyzing the clusters formed by the particles). This technique can be applied in DNS simulations to study turbulent reacting flows from a Lagrangian viewpoint, without excessive requirements for data storage.

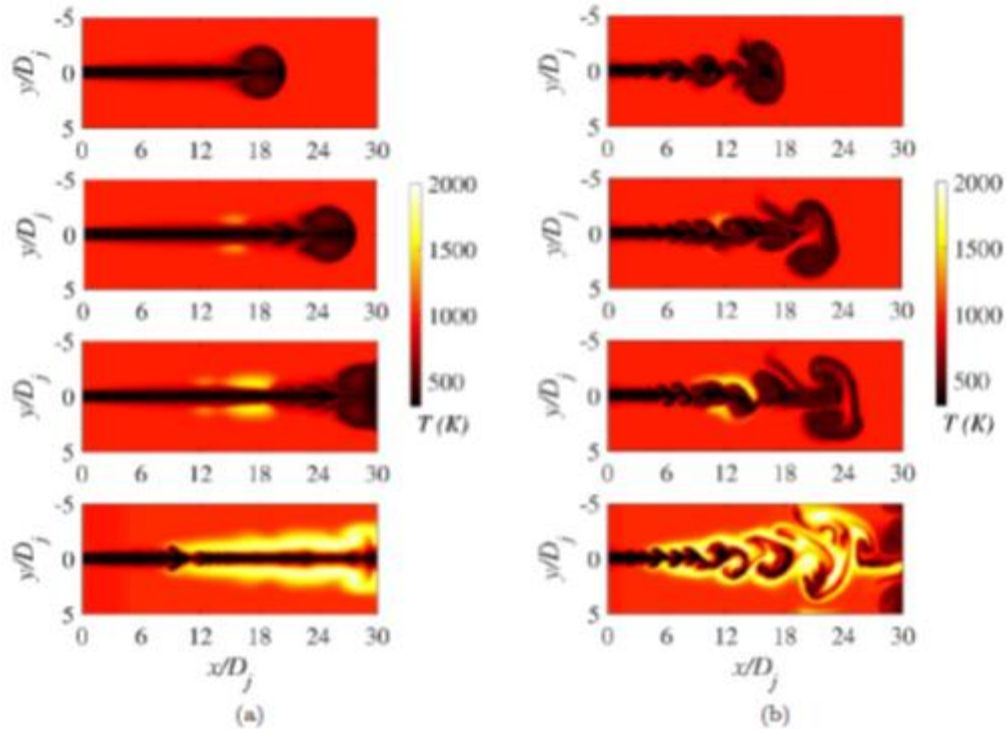
Flame particle tracking was used for various studies such as the evolution of individual points and surface elements in turbulent premixed flames. Figure 2 shows a temporally evolving flame front with embedded tracer particles in a typical simulation, elucidating the generation location and mechanism of the turbulent flame surface.



*Figure 2: Temporal evolution of the turbulent flame front with embedded tracer particles.*

Additionally, the response of flame speed to stretch rates was also investigated. The understanding of flame speed is important in developing models that have practical applications in understanding phenomena such as flashback in a combustor.

We performed a comparative study on the auto-ignition characteristics of a laminar hydrogen-nitrogen ( $H_2 - N_2$ ) jet issued into a co-flow of heated air, and wake of heated air (Figure 3).



*Figure 3: Instantaneous temperature contours for (a) Jet in a co-flow (b) Jet in a wake (JW) taken at interval  $t=0.5$  ms,  $0.675$  ms,  $0.75$  ms,  $1.0$  ms (from top to bottom)*

The work analyzed the relative roles of radical species in the initiation of auto-ignition process, and has applications in designing bluff body stabilized combustors.

- We also studied turbulence facilitated spark ignition of high Lewis number mixtures (rich hydrogen-air mixture). The study can lead to better understanding of the phenomenon and aid in the prediction of accidental explosion, optimization of engine flows for fuel-efficient operations, as well as understand the establishment of flame in a supernova explosion.

## Publications

1. Himanshu L. Dave, Abinesh Mohan, Swetaprovo Chaudhuri, “Genesis and Evolution of Premixed Flames in Turbulence”, presented at Asia-Pacific Conference on Combustion, held at the University of Sydney, Australia, 2017.
2. Abinesh Mohan, Himanshu L. Dave, Swetaprovo Chaudhuri, “Evolution of Surface Elements in Premixed Flames in Turbulence”, presented at Asia-Pacific Conference on Combustion, held at the University of Sydney, Australia, 2017.
3. Harshawardhan Uranakara, “Flame-Particle Tracking: Analysis of Turbulence-Premixed Flame Interaction (Doctoral dissertation).” Submitted in 2017.
4. Abinesh Mohan, “Lagrangian Flame-Element Analysis of Turbulence-Premixed Flame Interactions (Masters thesis).” Submitted in 2017.

# Chemistry

## Prof. Prabhu Nott's Lab

**Research Areas (details below):** Flow and handling of granular materials

**SahasraT Usage:** 2.1 million core hours

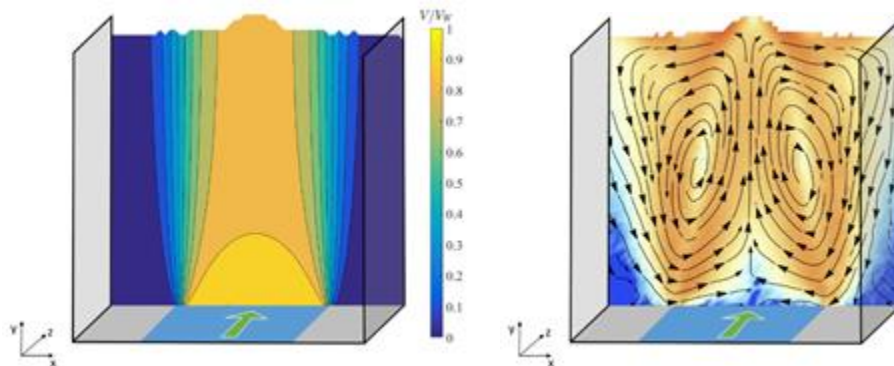
**Experimental Setup:** Up to 1032 cores of the Cray SahasraT compute nodes and the Dell visualization machine in SERC was used for the purpose. Open source molecular dynamics package Large Atomic Molecular Massively Parallel Simulator (LAMMPS) was used. The Message Passing Interface (MPI) was implemented using open source OPEN-MPI package.

**Performance:** The 1032 core job in CRAY executes in approximately 24 hours, which would otherwise take 5-7 days with resources available in our lab. Small and small72 jobs are too large to run locally.

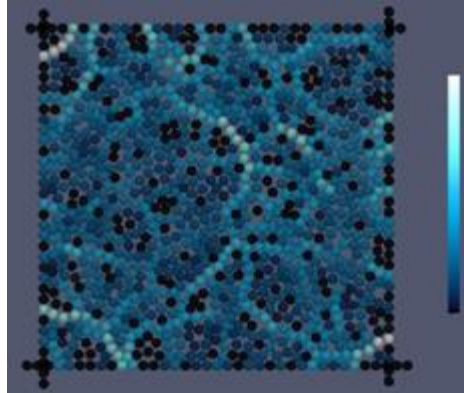
### Details of Research

#### Understanding Kinematics and Rheology of Granular Materials

The flow and handling of granular materials, such as foodgrains, ores and pharmaceutical powders, is important part of numerous industrial processes, yet fundamental understanding of their mechanics is lacking. To help develop such an understanding, we have studied the kinematics and rheology of granular materials by Discrete Element Method simulations. Additionally, such simulations have helped us understand certain topological features of grain clusters, called “force chains”, that are the agents of stress transmission.



*A granular material sheared in a split-bottom Couette cell, wherein a section of the base (blue) moves with velocity  $V_w$  relative to the stationary walls (grey), exhibits a dilation-driven secondary flow: (a) primary velocity ( $z$  direction), (b) secondary velocity in the  $x$ - $y$  plane.*



*Simulation of 2d isotropic compression of granular materials, the colours depicting the magnitude of force transmitted by grains (light colours meaning large force). The “force chains” that transmit large forces are apparent.*

### **Publications**

1. K. P. Krishnaraj and P. R. Nott, “A dilation-driven vortex flow in sheared granular materials explains a rheometric anomaly”, *Nature Commun.* 7, 10630 (2016).
2. P. V. Dsouza, K. P. Krishnaraj and P. R. Nott, Secondary flows in slow granular flows, *Powders and Grains* (2017).

# Climate Modeling

## Prof. Arindam Chakraborty's Lab

**Research Areas** (Details below): Study of Short-Term Weather Events

**SahasraT Usage:** 437,000 core hours

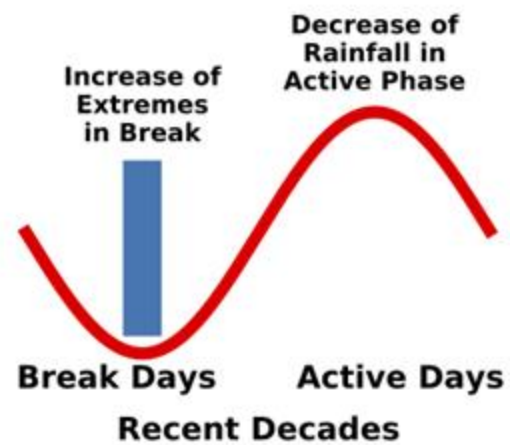
**Experimental Setup:** About 240 cores of ShasraT were used with a maximum of 24 cores per node.

**Performance:** It took about 4 hours to complete one year of real-time simulation.

### Details of Research

#### Study of Short-Term Weather Events

In this study we addressed how extreme (short-time) weather events modify (long-term) climate. The frequency of sporadic extremes rainfall events have increased significantly during past 7-decades. This is accompanied by decrease in the mean of Indian monsoon rainfall. Using several numerical simulations of a global general circulation model at the SERC's HPC system, we found that the increase in extremes was the cause of decrease in mean. Thus, for the first time we illustrate a mechanism that bridges short-term sporadic events to long-term means.



### Publications

1. Karmakar N, Chakraborty A, Nanjundiah RS. Increased sporadic extremes decrease the intraseasonal variability in the Indian summer monsoon rainfall. Scientific Reports. Nature Publishing Lab; 2017 Aug 10;7(1):7824.

## Prof. G Bala's Lab

### Research Areas (details below):

1. Simulation of water isotope ratios in rainfall
2. Climate modelling of geoengineering

**SahasraT Usage:** 542,000 core hours

**Experimental Setup:** About 128 cores of SahasraT were used. MPI distributed memory code was employed. For the first problem, for each simulation, 240 cores with an execution time of at-least 48 hours for each job submission are required. More than 20 such simulations were performed on Cray with plans to perform more simulations to complete the study.

For the second problem, CESM consists of five geophysical models: atmosphere, ocean, land, sea ice and land-ice, plus a coupler (cpl) that coordinates the models and passes information between them. The current model experiments use distributed memory parallelism implemented using MPI although shared memory parallelism option is also available in the model.

**Performance:** ~2.5-years/24 hours wall time. Similar performance was noted in HLRN in Hannover.

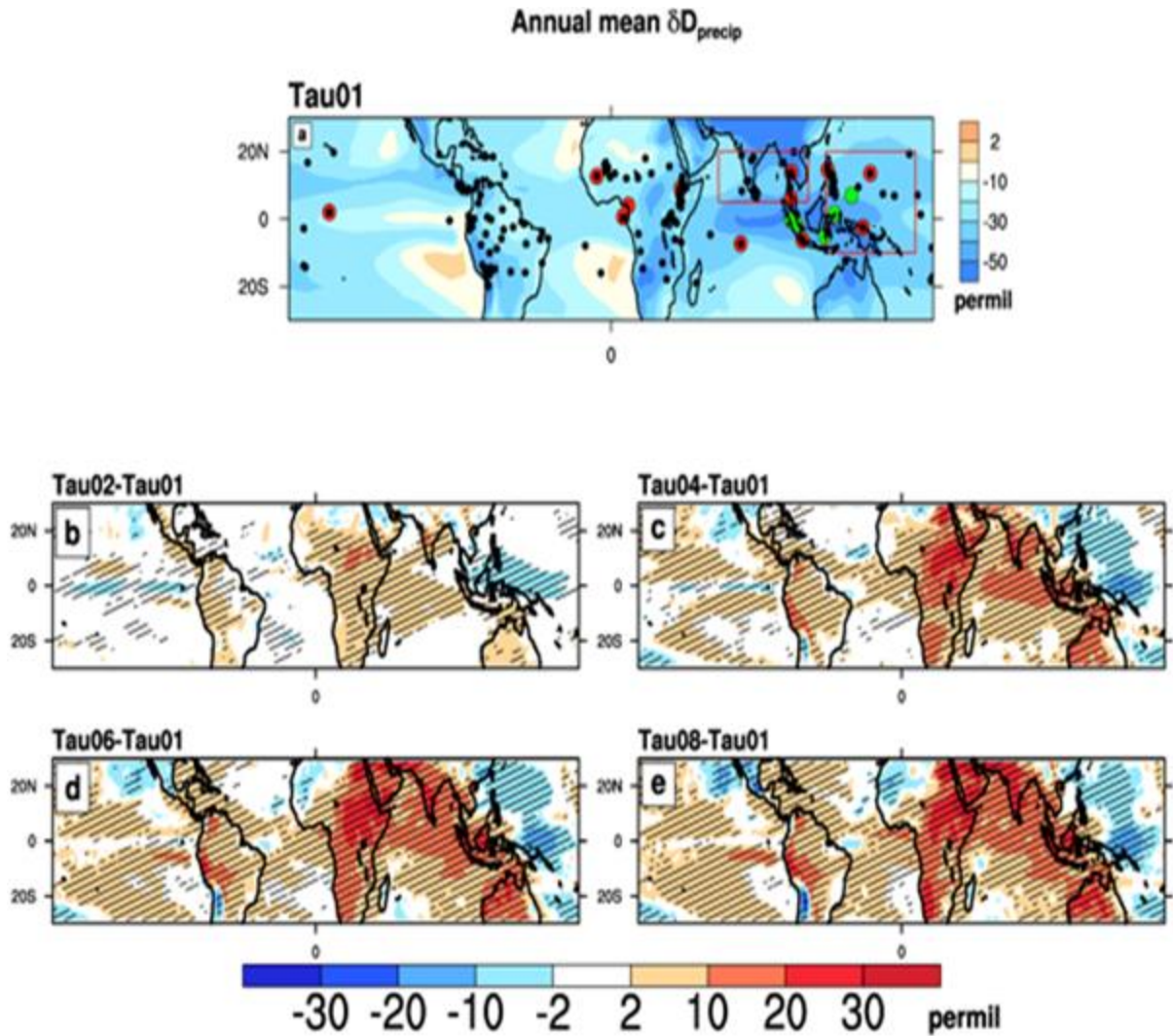
For the second problem, the earlier studies from the Lab were done in another cluster at the Center for Atmospheric and Ocean Sciences, IISc, called Mandhan. With the same model configuration, the cluster had a throughput of 12 model years in 24 hours using 96 cores. In Cray HPC we are getting a throughput of around 60 model years in 24 hours using 240 cores.

In one day, 18 years of model simulation are obtained. For the total simulation length of 250 years, it took about 2 weeks of wall clock time. For a typical research problem in the group, about 10 such 250-year long simulations are performed, equivalent to 20 weeks of wall clock time on 240 cores.

## Details of Research

### Simulation of Water Isotope Ratios in Rainfall

Simulation of present-day heavy water isotope ratio in tropical rainfall using an isotope-enabled climate model at a moderately high resolution (155km at equator). This study tested the sensitivity of the heavy isotope ratios in tropical rainfall to atmospheric deep convection.



*Figure: (a) Absolute annual mean values of heavy isotope ratios in precipitation ( $\delta D_{precip}$  in per mil) of the present-day baseline (Tau01) simulation. (b–e) The anomalies of annual mean  $\delta D_{precip}$  in per mil of the four sensitivity simulations (Tau02, Tau04, Tau06, and Tau08) in the tropics, relative to the baseline simulations where the amount of deep moist convection was reduced progressively. Regions where the anomalies are statistically significant at the 95% confidence level are hatched. It can be seen that the heavy isotope ratio increases as deep convection decreases. The multiple 20-year long equilibrium simulations for this study were performed on the SERC CRAY.*

## Climate Modeling of Geoengineering

Scientific knowledge on the proposed geoengineering methods to offset or reverse global warming scenario is of great interest to the scientific community. The proposed geoengineering methods propose to reduce the amount of sunlight that is absorbed by the planet. In Cray HPC, we are running geoengineering experiments using a global climate model CESM, where long-term numerical simulations are performed with prescribing sulfate aerosols in the stratosphere. These aerosols are known to scatter the solar radiation to space efficiently and cool the earth. In this study, the effects of particle sizes and aerosol

prescription height on changes in surface temperature and hydrological cycle are evaluated. These long-term simulations need to be run for hundreds of model years. The Cray HPC allows us to execute these experiments faster and helps to store and analyze the large volumes of output data (many terabytes) generated by the model.

**Video:** *Surface temperature anomaly on the planet for the period 1900-2100 (relative to the pre-industrial era). For the 21st century, a CO2 high emission scenario (RCP8.5) is used. The model used is the NCAR coupled climate model. These simulations were performed on SERC machines.*

## **Prof. PN Vinayachandran's Lab**

**Research Areas:** Understanding the role of river-runoff into oceans on climate

**SahasraT Usage:** 1.39 million core hours

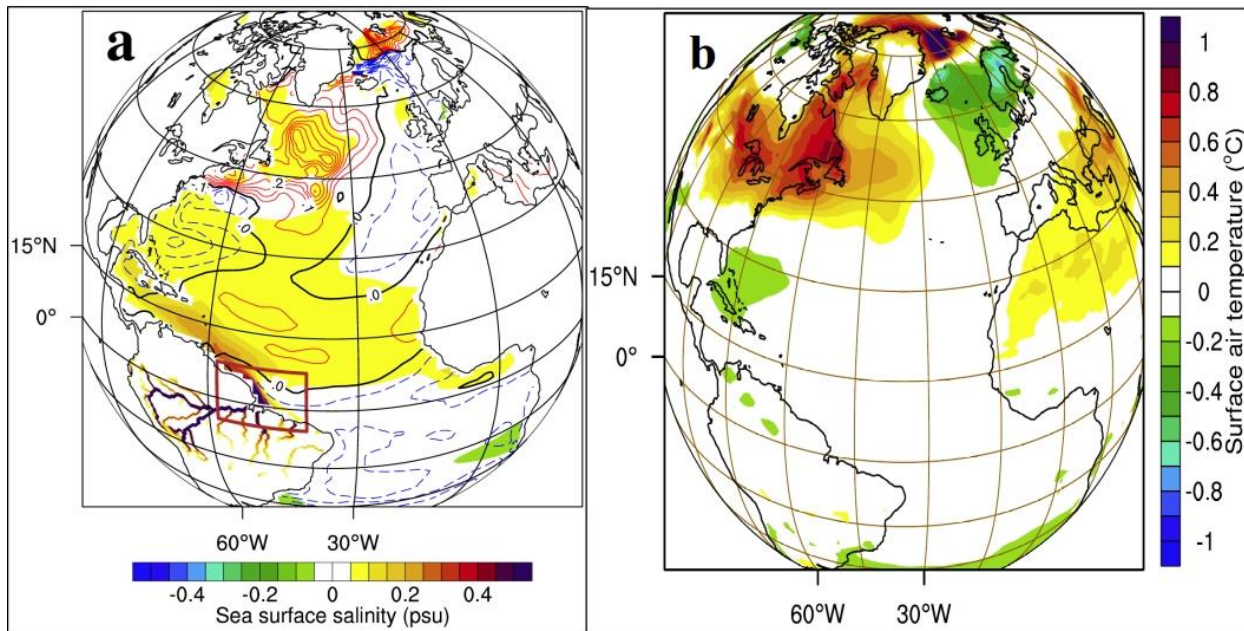
**Experimental Setup:** 1080 cores of SahasraT were used for the experiments. CESM is a parallel model that supports both MPI and OpenMP parallelism and for our model simulations in CRAY, we have employed Distributed Memory (DM) Parallelization using MPI. The parallel implementation is mainly done for the decomposition of the associated model spatial domain into two-dimensional blocks and the parallel input/output library (PIO) facility in CESM allows several processors to write individual records to the same file.

**Performance:** The jobs submitted in 'medium queue' (45 nodes and ncpus = 1080) for a 24-hour wall time gave a throughput of 12 model years. We have never tried these experiments on our local machines since it is a nearly impossible task.

### **Details of Research**

#### **Understanding the role of river-runoff into oceans on climate**

Our objective is to understand the role of river runoff into the ocean from major river systems like Amazon, Ganges-Brahmaputra, etc. on climate, using climate models. We use Community Earth System Model (CESM; version 1.2) and carry out 200 year long experiments by switching off river runoff into the ocean by individual and comparing them with the model run that includes the rivers. We find that the largest river controls the rainfall and temperature pattern over the Atlantic Ocean, Americas and Europe. The Ganga-Brahmaputra river system that discharges into the Bay of Bengal affects the rainfall pattern associated with the monsoons.



*Left panel: Response of the ocean to Amazon runoff. Amazon river network in the the model is shown in with a box (red lines) where the Amazon runoff into the ocean is intercepted in the model. Shading represents the increase in salinity in the absence of Amazon overlaid with contours representing corresponding change in temperature (°C) with black, red and blue contours indicating zero, increase, and decrease respectively.*

*Right panel: Atmospheric response in the absence of Amazon runoff. Mean winter (DJF) temperature increases (yellow and orange shades) over Eastern US, Arctic and Africa and decrease over parts of Europe (green and blue shades).*

## Publications

1. Jahfer, S., Vinayachandran, P. N. and Nanjundiah, Ravi S., 2017: Long-term impact of Amazon river runoff on northern hemispheric climate. *Nature Scientific Reports*, 7, 10989. doi:10.1038/s41598-017-10750-y.
2. Jahfer, S., Vinayachandran, P. N. and Nanjundiah, Ravi S., AMOC response to tropical Atlantic river runoff fluctuations, *Joint Assembly 2017*, 27 Aug-1 Sep 2017, Cape Town, South Africa.

# Materials Research Centre

## Prof. Abhishek Singh's Lab

**Team:** Himanshu Joshi, Anil Kumar Sahoo, Debabrata Pramanik, Biswajit Garai, Ipsita Basu, Mounika Gosika, Supriyo Naskar

**SahasraT Usage:** 14.4 million core hours

**Research Areas** (Details below): Novel topological materials

**Experimental Setup:** In most of the case, 240 cores were used. In some cases, greater than 1024 cores were also used. A parallel code VASP, Quantum Espresso and WannierTools were used, with both multicore and multinode parallelization.

### Performance

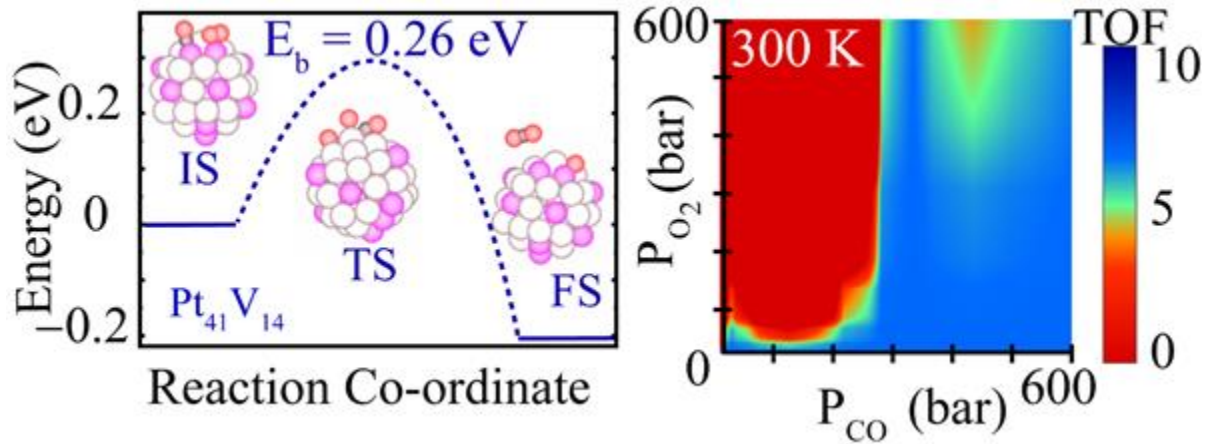
1. The computational facilities at SERC are much faster than the cluster. Typical execution times using SERC HPC systems were 24 hours or 72 hours. The same task would have taken at least an order of magnitude more time on the local facility.

### Details of Research

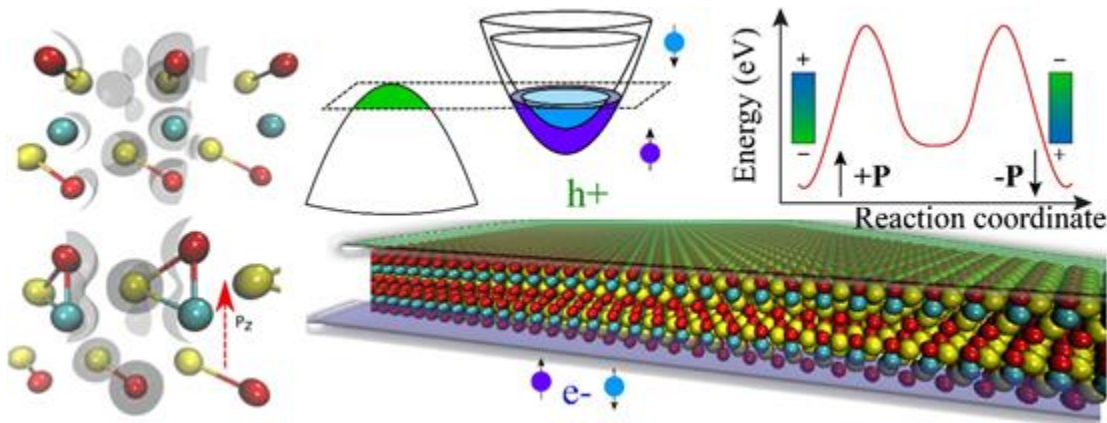
#### Discovering Novel Topological Materials

We have used SERC HPC facility for computational modelling of materials, especially in applications, where extensive computational resources were required. The main problems solved using this facility include the reaction barrier calculations, discovering novel topological materials and determining their exotic topological properties, calculating GW band gaps, evaluation of the anharmonic contributions to the lattice thermal conductivity of thermoelectric materials, and the determination of polarization of ferroelectric materials.

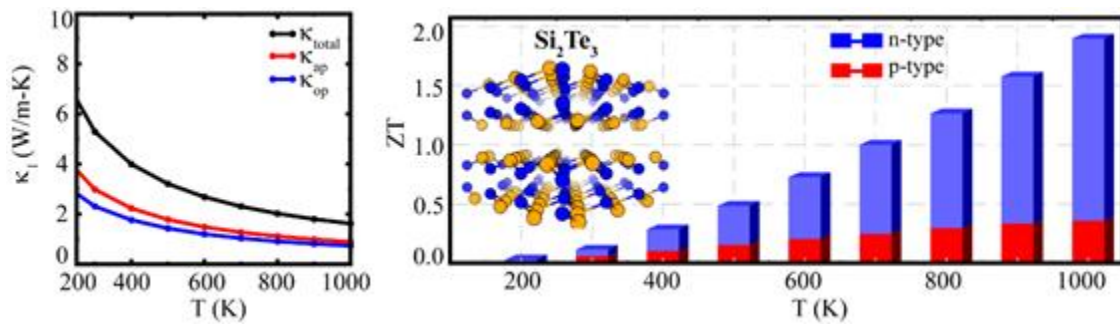
Reaction barrier and turn over frequency on 55 atom cluster supported on MgO (100)



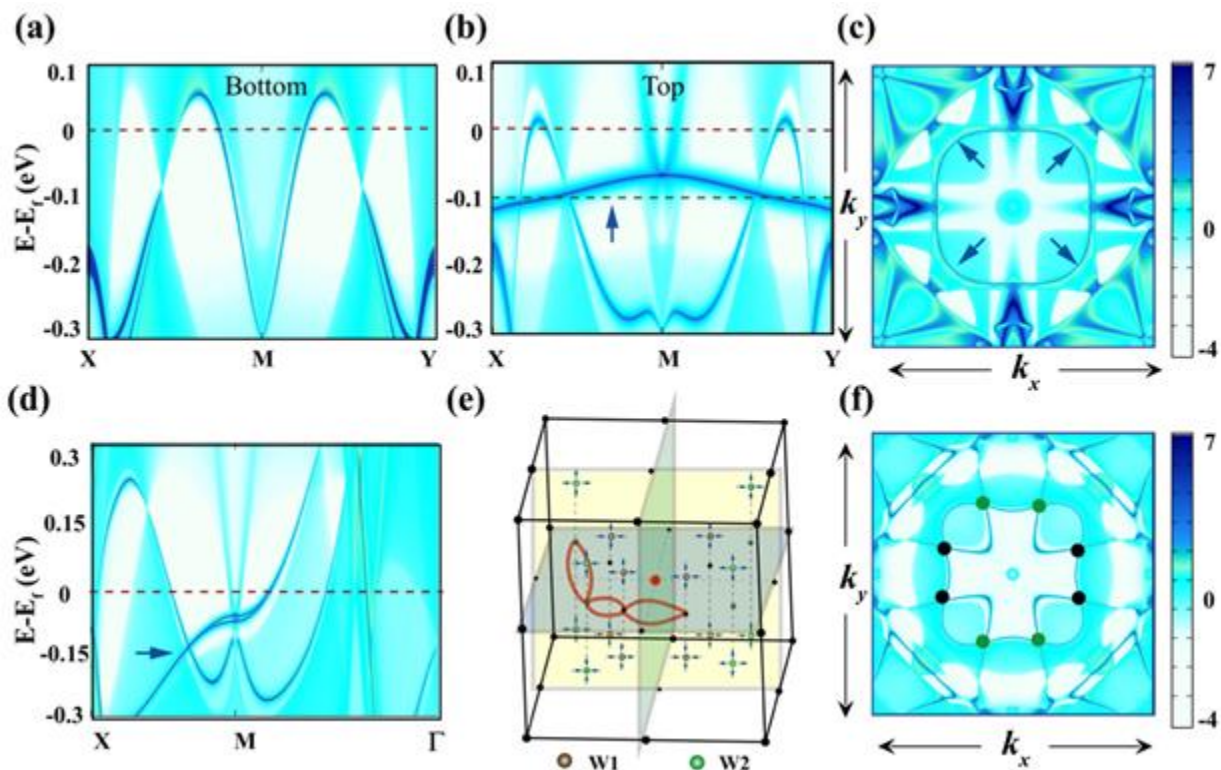
Ultra-thin 2D electron/hole gas in multi-functional monolayer MXene  $\text{Sc}_2\text{CO}_2$



Low thermal conductivity and very high figure of merit thermoelectric  $\text{Si}_2\text{Te}_3$



## Topologically non-trivial states in CaSn<sub>3</sub>



## Publications

1. Simultaneous site adsorption shift and efficient CO oxidation induced by V and Co in Pt Catalyst, R. Ahmad and A. K. Singh, *J. Phys. Chem.*, **121**, 12807 (2017)
2. Topologically nontrivial electronic states in CaSn<sub>3</sub>, S. Gupta, R. Juneja, R. Shinde, and Abhishek K. Singh, *J. Appl. Phys.* **121**, 214901 (2017)
3. High Thermoelectric Performance in n-doped Silicon-Based Chalcogenide Si<sub>2</sub>Te<sub>3</sub>, R. Juneja, T. Pandey and A. K. Singh, *Chem Mater.* **29**, 3723 (2017)
4. Ferroelectricity, Antiferroelectricity and Ultrathin 2D Electron/Hole Gas in Multifunctional Monolayer MXene, A. Chandrasekaran, A. Mishra, and A. K. Singh, *Nano Lett.*, **17**, 3290 (2017)
5. Strain-induced indirect to direct band gap transition in bulk SnS<sub>2</sub>, B. Ram and A. K. Singh, *Phys. Rev. B*, **95**, 075134 (2017)
6. Atomistic Origin of Phase Stability in Oxygen Functionalized MXene: A Comparative Study, A. Mishra, P. Srivastava, A. Carreras, I. Tanaka, H. Mizuseki, K.-R. Lee, and A. K. Singh, *J. Phys. Chem. C*, **121**, 18947 (2017)
7. Monolayer BC<sub>2</sub>: an ultrahigh capacity anode material for Li ion batteries, D. Das, R. Hardikar, S.-S. Han, K.-R. Lee, and A. K. Singh, *Phys. Chem. Chem. Phys.*, **19**, 24230 (2017)

8. Existence of  $Ti^{2+}$  states on the surface of heavily reduced  $SrTiO_3$  nanocubes, S. Shetty, S. K. Sinha, R. Ahmad, A. K. Singh, G. Van Tendeloo, and N. Ravishankar, *Chem. Mater.*, 29, 9887 (2017)
9. Graphene Oxide Epoxy (GO-xy): GO as Epoxy Adhesive by Interfacial Reaction of Functionalities, S. Vinod, C. S. Tiwary, A. Samanta, S. Ozden, T. N. Narayanan, R. Vajtai, V. Agarwal, A. K. Singh, G. John, and P. M. Ajayan, *Adv. Mater. Interfaces*, 1700657 (2017)
10. Towards Band Structure and Band Offset Engineering of Monolayer  $Mo_{(1-x)}W_xS_2$  via Strain, J.-S. Kim, R. Ahmad, T. Pandey, A. Rai, S. Feng, J. Yang, Z. Lin, M. Terrones, S. Banerjee, A. K. Singh, D. Akinwande, and J.-F. Lin, *2D Materials*, 5, 015008 (2017)
11. Manipulation of Opto-electronic Properties and Band Structure Engineering of Ultrathin Te Nanowires by Chemical Adsorption, A. Roy, K. R. Amin, S. Tripathi, S. Biswas, A. K. Singh, A. Bid, and N. Ravishankar, *ACS Appl. Mater. Interfaces*, 9, 19462 (2017)
12. Negative differential resistance in armchair silicene nanoribbons, A. Manjanath, A. Roy, A. Samanta, and A. K. Singh, *Nanotechnology*, 28, 275402 (2017)
13. Orientation Selection During Heterogeneous Nucleation: Implications for Heterogeneous Catalysis, D. Chatterjee, A. Reghunath, K. Kamalnath, R. Ahmad, A. K. Singh, and N. Ravishankar, *J. Phys. Chem. C*, 121, 10027 (2017)
14. Growth of Molybdenum Carbide-Graphene Hybrids from Molybdenum Disulfide Atomic Layer, J. Wu, L. Ma, A. Samanta, M. Liu, B. Li, Y. Yang, J. Yuan, J. Zhang, Y. Gong, J. Lou, R. Vajtai, B. Yakobson, A. K. Singh, C. S. Tiwary, P. M. Ajayan, *Adv. Mater. Interfaces*, 1600866 (2017)
15. One-Step Electrodeposited 3D-Ternary Composite of Zirconia nanoparticles, rGO and PolyPyrrole with Enhanced Electrochemical Performance, A. P. P. Alves, R. Koizumi, A. Samanta, L. D. Machado, A. K. Singh, D. S. Galvao, C. S. Tiwary, G. G. Silva and P. M. Ajayan, *Nano Energy*, 31, 225 (2017)
16. Utilizing metal immiscibility to create two-dimensional metal carbide, boride and nitrides on Copper, Z. Wang, V. Kochat, P. Pandey, S. Kashyap, S. Chattopadhyay, A. Samanta, S. Sarkar, P. Manimunda, X. Zhang, S. A. Asif, A. K. Singh, K. Chattopadhyay, C. S. Tiwary, P. M. Ajayan, *Adv. Mater.*, 1700364 (2017)
17. Insights into Nucleation, Growth and Phase Selection of  $WO_3$ : Morphology control and Electrochromic Property, K. Ghosh, A. Roy, S. Tripathi, S. Ghule, A. K. Singh, and N. Ravishankar, *J. Mater. Chem. C*, 5, 7307 (2017)
18. Fluorinated h-BN as magnetic semiconductor, S. Radhakrishnan, D. Das, A. Samanta, C. Reyes, L. Deng, L. B. Alemany, T. K. Weldeghiorghis, V. N. Khabashesku, V. Kochat, Z. Jin, P. M. Sudeep, A. A. Martí, C.-W. Chu, A. Roy, C. S. Tiwary, A. K. Singh, P. M. Ajayan, *Science Advances*, 3, e1700842 (2017)

# Microbiology and Cell Biology

## Prof V Nagaraja's

**Research Areas** (Details below): Functional differences of proteins.

**SahasraT Usage:** 373,320 core hours

**Experimental Setup:** Tyrone cluster was used with 256 cores for 240 hrs wall time (approximately) and Cray system was used for 360 hrs wall time with 2112 cores approximately. Dell Visualisation Server was used for post processing of the results. Mvapich2 was used for parallelisation purpose.

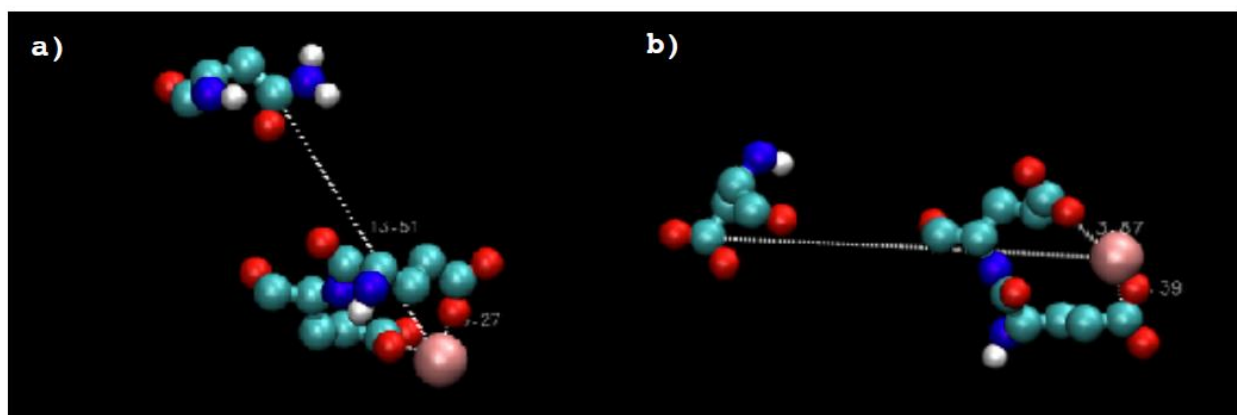
## Performance and Problem Size

On the basis of wall time for a job execution Tyrone cluster is approximately 8 times faster compared to our system and Cray is beyond comparison. Both of them are also far better than our system in terms of precision and accuracy of the result.

## Details of Research

### Functional Differences of Proteins

We are interested in the basis of functional differences of two similar proteins in Mycobacterium tuberculosis. Alteration of a few amino acid residues leads to reversion of functionality of one protein and make it more like other. But biochemical analysis show that their mode of actions are different than each other. Molecular dynamics simulation study has been used to look further into this differential mode of actions of those proteins.



**Fig.:** Distances of Mg ion from various amino acid residues in a) mut5-d45n mutant, b) mut5-Rv3788 after molecular dynamics simulation

# Mechanical Engineering

## Prof. Raghuraman Govardhan's Lab

**Research Areas** (Details below): Study of Unsteady Thrust Generation Systems.

**SahasraT Usage:** 6.34 million core hours

**Experimental Setup:** About ten K-40 GPU cards on the Cray SahasraT system were used for the experiments. We utilize a high-resolution GPU-accelerated viscous vortex particle method for simulation of fluid-structure interaction problem associated with pitching foil configuration. The method relies on vortex blobs for flow field representation and hence problems similar to the well-known N-Body problem are encountered about 8 times per time step of flow evolution. In our implementation we use the Fast Multipole Method to reduce the time complexity of the N-Body algorithm from  $O(N^2)$  to  $O(N)$ .

### Performance and Problem Size

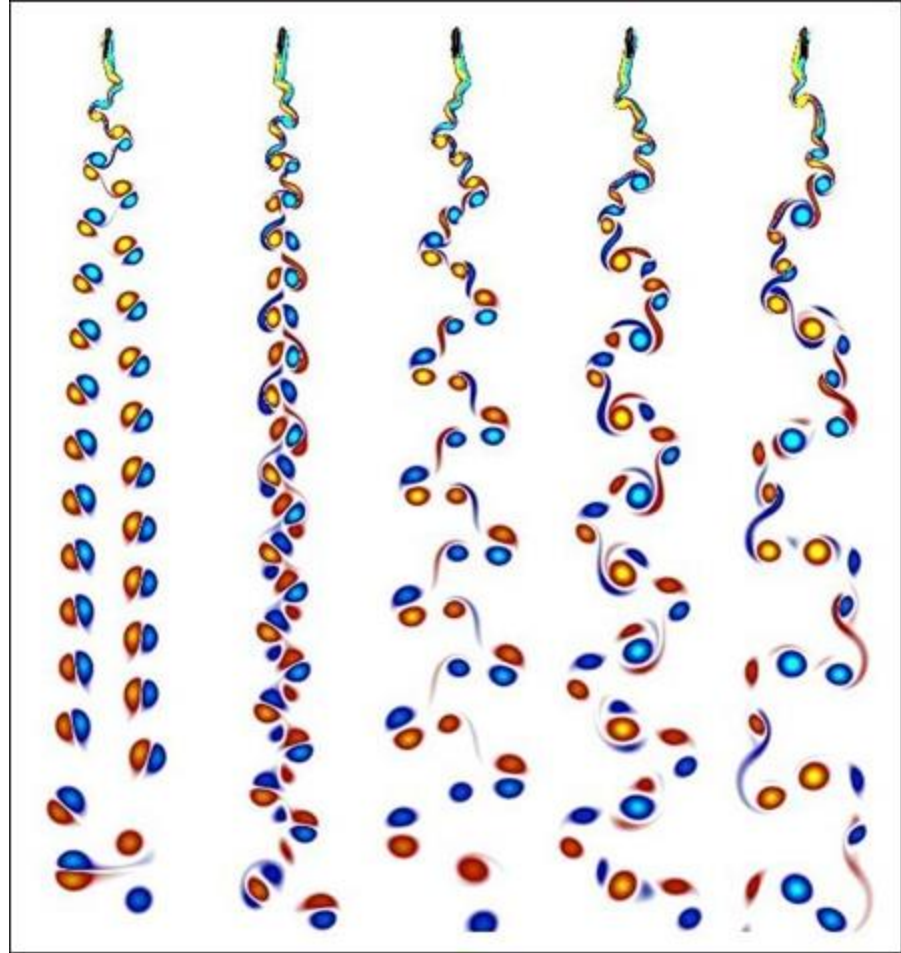
Our test runs indicate that compared to conventional implementation on multicore CPU architectures our GPU-accelerated implementation allow us to perform computations on thousands of cores that are available on modern general purpose graphics processing units and thus achieve over an order of magnitude speed up (compared to an OPENMP implementation on 12 cores we observe over a ten fold speed up using a single Tesla K40 GPU with 2880 cores).

### Details of Research

#### Study of Unsteady Thrust Generation Systems

The recent thrust on miniaturization of micro air vehicles and unmanned air vehicles has necessitated a reanalysis of the conventional steady thrust generation systems and new look into unconventional unsteady

ones. Conventional thrust generation systems rely on fixed wings for generating the thrust and lift necessary for forward flight and rapidly lose their efficacy at small sizes. In contrast, unsteady flapping wing configurations find widespread prevalence in animal locomotion. It is therefore important to investigate unconventional unsteady thrust generating mechanisms that are typically observed in nature. In this work we aim to develop an advanced understanding of the unsteady thrust generation from a biomimetic unsteady pitching foil configuration. Our overarching objective is a feasibility analysis and optimization of this configuration for eventual utilization in micro air vehicle/unmanned air vehicle propulsion.



*Figure illustrates the different wake patterns (2P, 2P+2S, 2P+2S2, 4P and 4P+2S from left to right, where S and P denote a single vortex and counter rotating vortex pair, respectively) generated from variations in pitching angle and amplitude of a foil flapping in a uniform free-stream. These multi-million GPU-accelerated viscous vortex particle simulation runs were performed on a single Tesla K40 GPU with 2880 cores.*

## **Publications**

- 1) A. Das, R.K. Shukla, and R.N. Govardhan, Self-propulsion of a pitching foil, Bulletin of the American Physical Society, 2017, 70th Annual Meeting of the APS Division of Fluid Dynamics Volume 62, Number 14.

## Prof. Ratnesh Shukla's Lab

**Research Areas** (Details below): Hydrodynamics

**SahasraT Usage:** 26.9 million core hours

**Experimental Setup:** About 7200 cores of Cray ShasraT were used. We utilize a high-resolution, MPI-parallelized incompressible flow solver that relies on high-order accurate compact finite-difference discretization along wall-normal or aperiodic, and Fourier spectral discretization along periodic directions. To achieve high parallel performance, our implementation employs domain decomposition and an influence matrix technique in a way that minimizes intra-node communication.

### Performance and Problem Size

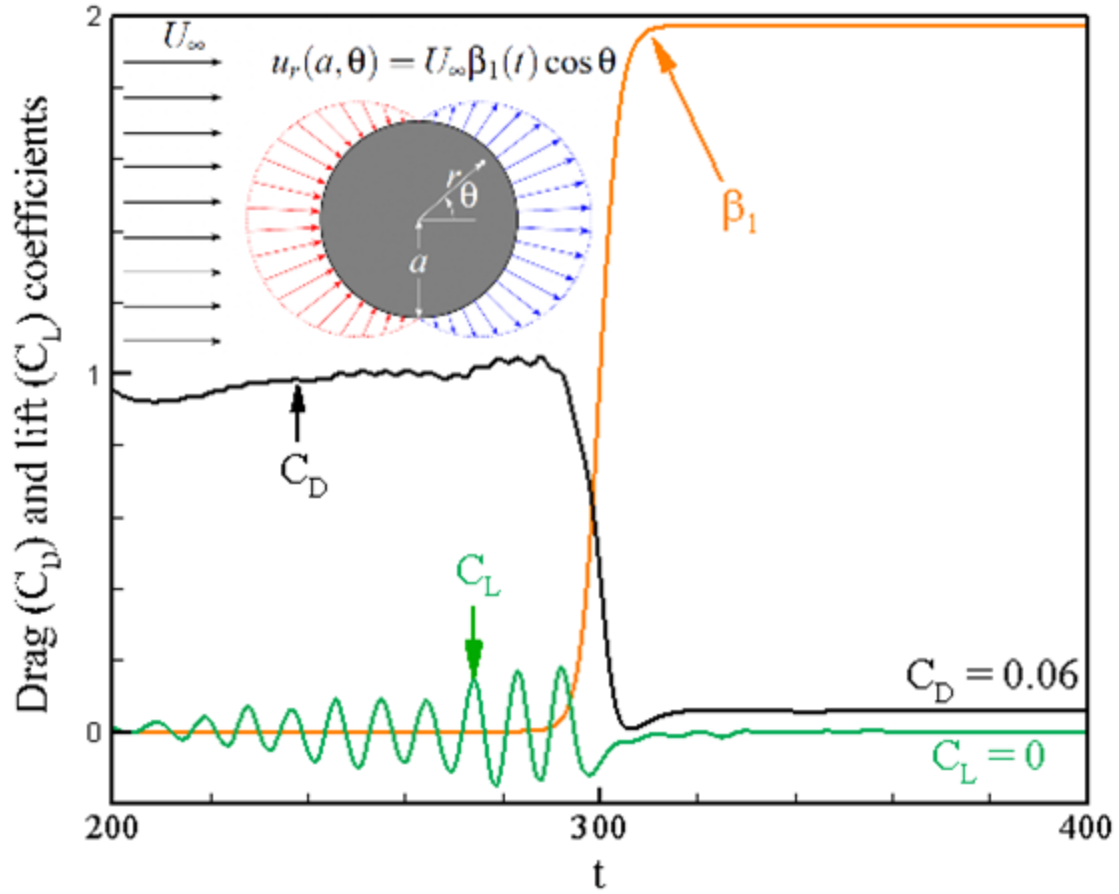
Numerical tests indicate that our high-order accurate flow solver yields excellent scalability up to about ten thousand cores on the CRAY XC-40 computing platform. The problems we are currently simulating using CRAY XC-40 are out of reach of our modest scale computing resources that typically consist of only a few hundred cores.

## Details of Research

### Hydrodynamics

Our objective is to develop an advanced understanding of the influence of hydrodynamic slip on the flow and transport characteristics through direct numerical simulations. Through an effective suppression of vorticity production at the solid surface, hydrodynamic slip is known to enable significant drag reduction over a variety of planar and bluff-body flow configurations. This reduction can lead to substantial power savings in prototypical flow configurations. An understanding of the influence of textured surface enabled slip on flow and transport characteristics is therefore of significant fundamental and technological importance.

Application of wall-normal blowing & suction results in decrease in hydrodynamic loads on a translating circular cylinder. The attached movie shows reduction in the generation of vortical structures and their advection after flow control is activated.



### Publications

1. N. M. A. Rehman, A. Kumar, and R. K. Shukla, Influence of hydrodynamic slip on convective transport in flow past a circular cylinder, *Theoretical and computational fluid dynamics*, Vol. 31(3), pp. 251-280.
2. K. S. Patel and R. K. Shukla, Numerical simulation of breakup and detachment of an axially stretching Newtonian liquid bridge with a moving contact line phase field method, *Sadhana*, Vol. 42(4) pp 467-477.

# Physics

## Prof. Chandan Dasgupta's Lab

### Research Areas:

1. Molecular dynamics simulation of glass forming systems
2. Molecular dynamics simulation of active glass
3. Numerical computation of thermal properties of glasses

**SahasraT Usage:** 3 million core hours

**Experimental Setup:** SahasraT up to 5000 cores were used for parts of the work. Home-grown codes were parallelized using MPI.

### Performance

For some of the work, maximum allowed execution time queue of 72 hours was used. With the same number of cores, we have observed a speed-up of about 2.5-3 times as compared to the runs in “Rahman” cluster of the Physics department. With the same number of cores, we have observed a speed-up of about 2.5-3 times as compared to the runs in “Rahman” cluster of the Physics department.

### Publications

1. Thermal Conductivity of Glass-Forming Liquids (arXiv:1703.04494)
2. Glassy swirls of active dumbbells (Phys. Rev. E 96, 042605)
3. Activity controls fragility: A Random First Order Transition Theory for an active glass (arXiv:1605.06073)

## Prof. Prabal Maiti's Lab

**Team:** Himanshu Joshi, Anil Kumar Sahoo, Debabrata Pramanik, Biswajit Garai, Ipsita Basu, Mounika Gosika, Supriyo Naskar

**Research Areas** (Details below): DNA Nanotechnology, nanomedicine and gene therapy, study of dendrimers, fusion of HIV gp41, protein synthesis, study of nanotubes

**SahasraT Usage:** 12.88 million core hours

**Experimental Setup:** For all these simulations, 8 nodes (172 cores) to 50 nodes (1200 cores) of CPU on Cray SahasraT were used. In the simulations related to DNA nanotechnology, two GPU nodes were used. MPI, MVPICH, Charm++ based parallelizations were employed. Software packages including AMBER, NAMD, LAMPPS, Quantum Espresso and GROMACS were used. In one case related to study of nanotubes, GPU version of PMEMD was used.

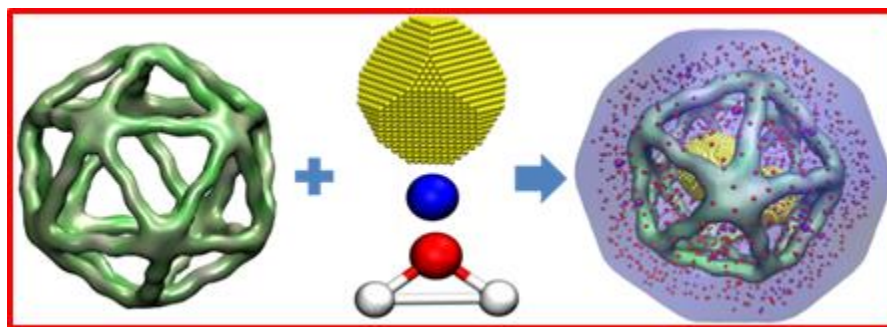
## Performance

1. NAMD codes were quite efficient on Cray CPUs.
2. CUDA version AMBER was also very fast on Cray GPUs.
3. In many cases, the use of SahasraT Cray systems yielded at least 2X performance improvement over the use of the local systems.
4. In one case, around five times higher performance was obtained with the Cray system (10ns/day) compared to the lab system (2ns/day) for a system of about 0.3 million atoms (for NAMD simulation tool). Scaling with AMBER simulation tool is about 3 times as compared to the system.
5. In one case related to study of nanotubes, the performance was 7 to 8 nanoseconds per day for around 2.5 lakh atoms.

## Details of Research

### DNA Nanotechnology

DNA nanotechnology is a rapidly emerging field which enables a route to create functional sub-micron size nanomachines. In order to control the efficient design and behavior, it is imperative to understand their nanoscale properties. We have performed extensive all-atom MD simulation of self-assembled nanostructures such as transmembrane DNA nanopores and DNA icosahedron, using the SERC HPC resources to predict their structural, mechanical and electrical properties. Our simulation has been complementary to realize vDNA nanostructure for in-vivo applications. Our membrane protruding DNA nanopores simulation partially explained the stability of these complex nanopores and provide a theoretical basis to their insertion mechanism.



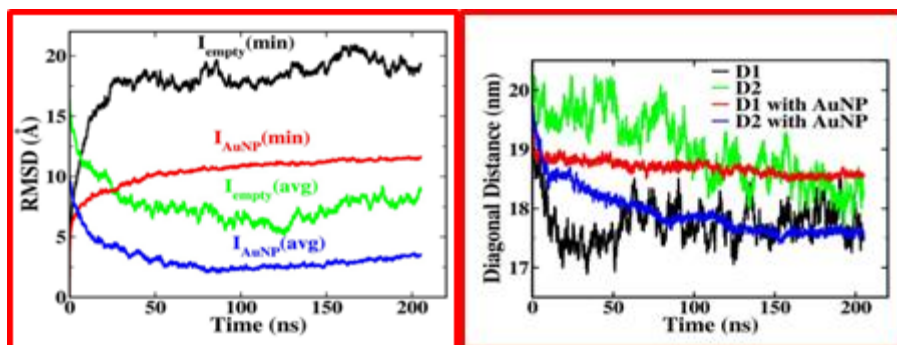


Figure : All atom model of cargo loaded DNA icosahedron, the system contains  $\sim 1$  million atoms including the water and ions. The MD simulation of this structure was one of the largest all atom simulations ever realized considering the length of simulation time and number of atoms. (a) (left) Empty  $I_{DNA}$ , (right) solvated and charge neutralized structure of AuNP encapsulated  $I_{DNA}$ . (b) The time evolution of the RMSD of  $I_{DNA}$  with respect to the initially minimized structure and also with respect to the average structure over the last 50 ns long simulation. (c) Two distinct diagonal distance of  $I_{DNA}$  with respect to the simulation time. The analysis shows the additional stability of cargo loaded  $I_{DNA}$  as compared to the empty  $I_{DNA}$ .

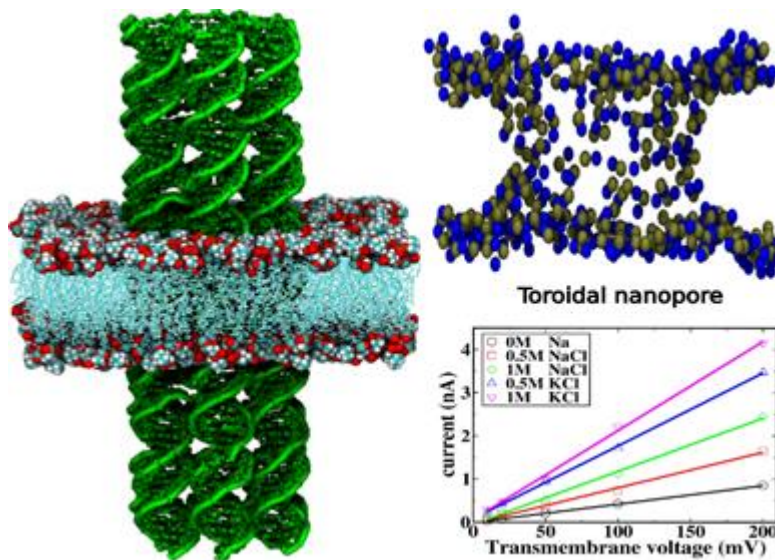


Figure: Transmembrane DNA nanopore (left) simulated in atomistic simulation. The snapshots of the polar atoms of the head Labs of lipid bilayer after 200 ns of MD simulation (top left figure) shows the formation of toroidal transmembrane nanopore. The bending of Lipid head Labs cooperatively account for the in-silico stability of self-assembled transmembrane DNA channels. Transmembrane ionic current traces as a function of applied voltages for various salt concentrations. This image has been selected for the cover image of upcoming issue of journal Nucleic Acid Research.

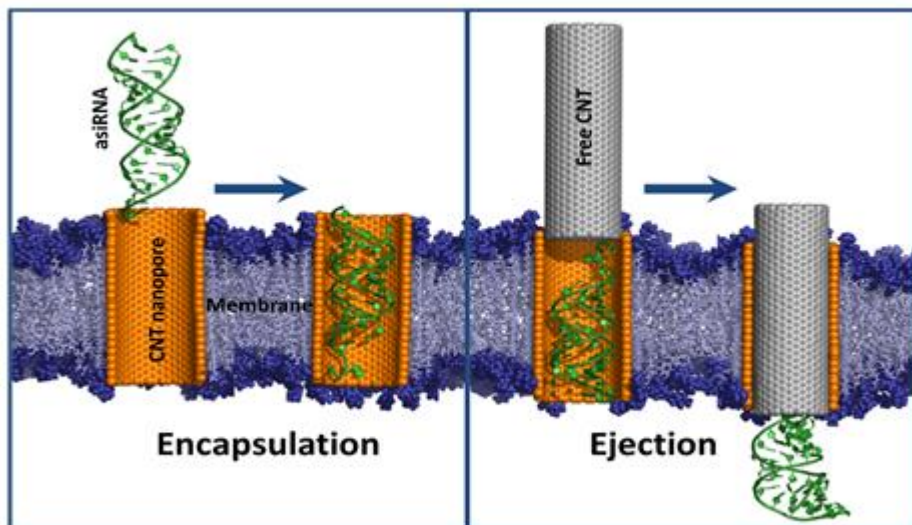
## Videos

**Video V1:** Dynamics of DNA icosahedron in explicit salt solution (contacting 780841 atoms) during the course of 205 ns MD simulation, the ions and water are not shown in the movie.

**Video V2:** Typical simulation movie of 0.2  $\mu$ s long MD simulation trajectory of system in 1M NaCl electrolyte solution. Water atoms are not shown.

## Nanomedicine and Gene Therapy

One of the major challenge of the nanomedicine and gene therapy is the effective translocation of drugs and genes across cell membranes. Generally, the bioactive molecules used for this purpose cannot passively pass through the cell membrane due to very high penalty associated with membrane rupture. We propose a carbon nanotube based technology that can translocate bioactive molecules into the cell. Using molecular dynamics simulation, we show that molecules of various shape, size, and chemistry can be translocated across a model lipid bilayer membrane following our protocol, as we have exemplified with dendrimers, asiRNA, ssDNA and ubiquitin protein. This method should work for other molecules as well, and hence could be potentially useful for drug delivery application.



*Figure: Protocol for translocation of asiRNA across a model lipid membrane bilayer. (Left) Snapshots from molecular dynamics simulation show that an asiRNA molecule can spontaneously enter a stable CNT-nanopore embedded in the lipid bilayer membrane. (Right) A freely floating CNT insert spontaneously into the nanopore, and hence displaces the encapsulated asiRNA out of the nanopore. So, the above method can be used to transfer asiRNA as well as other bioactive molecules across the cell membrane, which otherwise would not have been possible because of very high free energy barrier for membrane rupture.*

## Videos

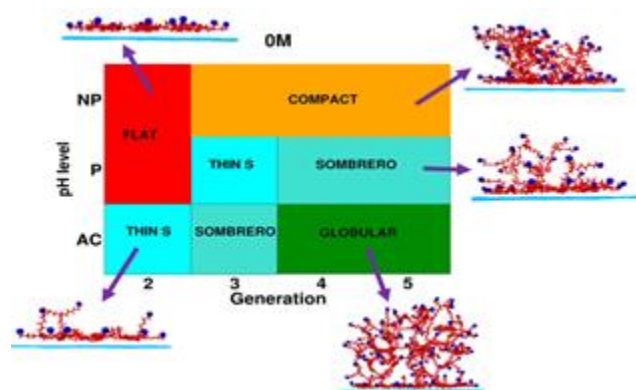
**Video V1:** Spontaneous encapsulation of the asiRNA molecule inside the CNT nanopore embedded in the lipid bilayer membrane.

**Video V2:** Ejection of the encapsulated asiRNA molecule using a small diameter CNT, which can spontaneously enter inside the CNT nanopore due to its strong VDW attraction energy with the nanopore and displaces the encapsulated molecule outside the nanopore.

## Study of Dendrimers

To estimate the efficiency of the dendrimer for the dispersion of CNTs from the bundle geometry, we have calculated potential of mean forces (PMF) for non-protonated, and protonated dendrimer with three different generations (2 to 4) and showed the effective dispersion efficiency for various systems.

We also studied the interaction of mannose dendrimer with single-walled carbon nanotube (SWCNT) using all-atom molecular dynamics (MD) simulations. Our all-atom MD simulations demonstrate that mannose dendrimer wraps around SWCNT of various chiralities and forms a nice composite structure. From our DFT based calculations, we have confirmed that when a metallic CNT is wrapped by Mannose dendrimer, a metallic-semiconducting transition is observed.



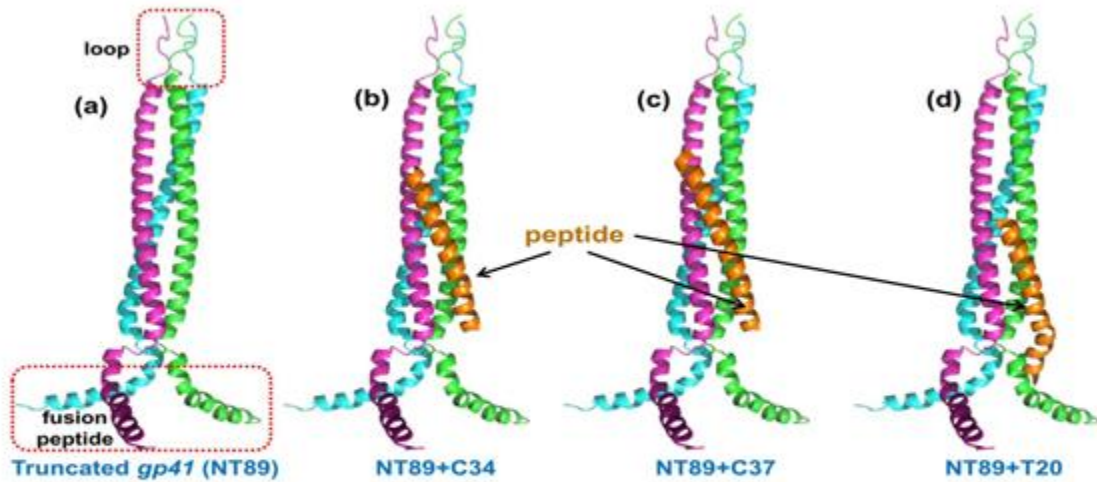
pH dependent adsorption of PAMAM dendrimers on graphene is interesting for various applications such as drug delivery, supercapacitors, surface patterning etc. Molecular Dynamics Simulations are the best way to probe the conformational changes in the structures of these dendrimers. A part of the problem is to investigate the binding energy strengths of the dendrimer-graphene composites as a function of pH level of the surrounding medium.

*Figure: Morphology map of the PAMAM dendrimers on graphene as a function of pH and generation number. Some of these morphologies are analogous to adsorbed star-polymer morphologies.*

## Fusion of HIV gp41

The fusion mechanism of HIV gp41 is not well understood despite several decades of experimental research. In this context, molecular dynamics simulations of complex human and HIV membrane models were performed to explore the mechanism with molecular details. The rate of lipid mixing/fusion of human and HIV membrane can be predicted from simulations performed at varying temperatures. Inhibitors to

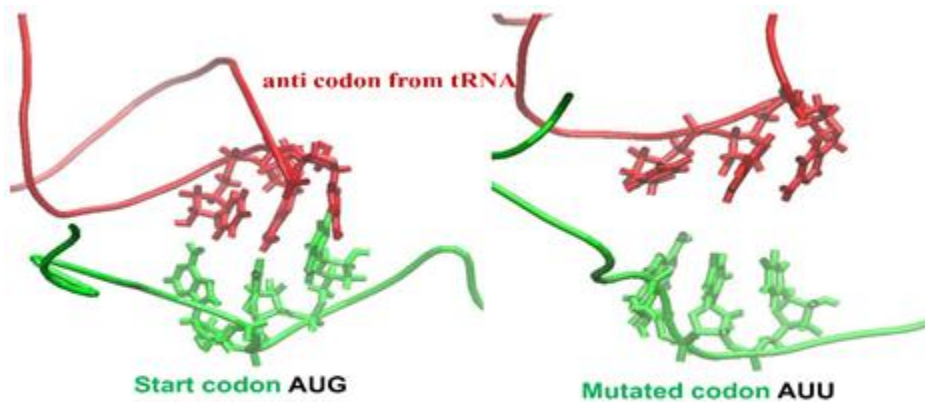
eradicate the fusion will be designed further and various thermodynamic parameters will be obtained using computational approaches.



**Figure: Complex of HIV-1 gp41 (cyan, green and magenta helices) with peptide inhibitors (orange helix) C34 (b), C37 (c) and T20 (d) subjected to simulations studies. Position restraints applied to regions of gp41 are shown with red dotted box (a) and explicit water molecules are not shown for clarity.**

### Protein Synthesis

In order to start the initiation of translation in eukaryotic protein synthesis in the ribosome, the correct start codon has to be recognized. The tRNA binds to the mRNA and scanning is started until the correct start codon AUG is found. There is a controversy in this process whether tRNA can scan the codons when the ribosome is in open state or it has to go to closed state for each codon scanning. So from the energetic landscape of base pairing between tRNA and different near cognate codons in mRNA in both states, the scanning ability of tRNA can be explored.



**Figure: Codon–anticodon binding interaction for the start codon and one mutated codon**

## Study of Nanotubes

In this work, we study the effect of ion concentration on hexagonal nanotubes made of 6 double-stranded DNA. Utilizing all-atom molecular dynamics study over several hundred nanoseconds in the presence of explicit water and ion, we get a fundamental insight of the microscopic structure, conformational change, and interaction of the DNA nanotubes with the external environment. We quantify various structural aspects of the nanotubes and how they change with the salt concentration.

### Publications:

1. Structure and electrical properties of DNA nanotubes embedded in lipid bilayer membranes, H Joshi, PK Maiti . *Nucleic Acid Research* **2017**.
2. Probing the structure and in silico stability of cargo loaded DNA icosahedra using MD simulations H Joshi, D Bhatia, Y Krishnan, PK Maiti. *Nanoscale*, **2017**, 9 (13), 4467-4477.
3. Anil Kumar Sahoo, Subbarao Kanchi, Taraknath Mandal, Chandan Dasgupta and Prabal K. Maiti, Translocation of Bioactive Molecules through Carbon Nanotubes Embedded in Lipid Membrane, *ACS Applied Materials & Interfaces*, 2018 (just accepted manuscript).
4. Dendrimer assisted dispersion of carbon nanotubes: a molecular dynamics study, D. Pramanik and Prabal K. Maiti; *Soft Matter*, 2016, 12, 8512-8520.
5. DNA assisted dispersion of carbon nanotubes and comparison with other dispersing agents, D. Pramanik and Prabal K. Maiti; *ACS Appl. Mater. Interfaces*, 2017, 9, 35287-35296.
6. Opening of large bandgap in metallic carbon nanotubes by mannose functionalized dendrimers: experiments and theory, K. S. Vasu, D. Pramanik, S. Kundu, N. Jayaraman, M. Jain, Prabal K. Maiti and A. K. Sood (under review).
7. Mannose dendrimer wrapping drives metal-semiconductor transition in carbon nanotubes, D. Pramanik, K. S. Vasu, M. Jain, A. K. Sood and Prabal K. Maiti (to be submitted).
8. pH and Generation Dependent Morphologies of PAMAM Dendrimers on Graphene, Mounika Gosika and Prabal K Maiti, (Under review in soft matter).

## Prof. Prateek Sharma's Lab

**Team:** Prakriti Pal Choudhury, Prasun Dhang, Siddhartha Gupta, Santosh Khetan, Rajsekhar Mohapatra, Deovrat Prasad, Aditi Vijayan, Naveen Yadav

**Research Areas** (Details below): Simulations of galaxy clusters, interacting supernovae

**SahasraT Usage:** 14.8 million core hours

**Experimental Setup:** We have mostly used SahasraT and the Dell visualization servers. Our core usage varies from 240 to ~10000, depending on the problem. We ran a scaling run on up to 16000 cores

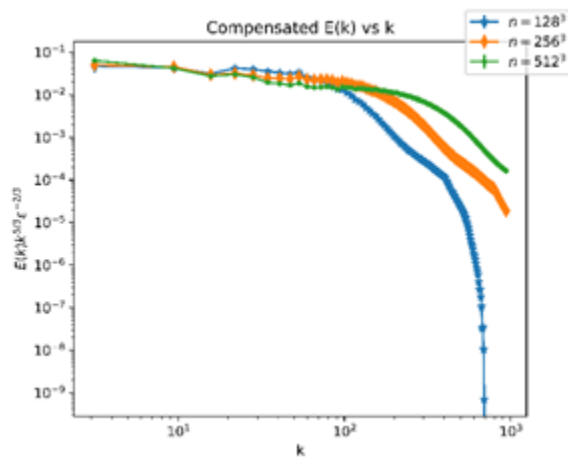
for showcasing a new explicit super-time-stepping algorithm for anisotropic thermal conduction. We use efficient parallel MHD codes PLUTO and ZEUS and add parallel modules to them according to our applications. We have tested scaling of our applications. We use MPI for parallelization.

## Performance and Problem Size

Our large runs are only possible on SahasraT. They cannot be done on our local clusters (the biggest of which is a 256-core machine). At times we have also requested time to run long jobs for a longer time on call from SERC.

## Details of Research

### Simulations of Galaxy Clusters, Interacting Supernovae



My Lab has used SERC's SahasraT cluster to solve important problems in astrophysics. We have performed state of the art simulations of X-ray emitting gas in galaxy cluster cores interacting with powerful jets driven by the central supermassive black holes. We have carried out hydrodynamic simulations of turbulence in cores of galaxy clusters. Another focus of our Lab is MHD simulations of local and global non-radiative accretion flows. We also work on the simulations of interacting supernovae going off in the interstellar medium. SahasraT has helped with the PhD thesis work of most of my students.

*Figure: Power spectrum of kinetic energy from*

*isotropic homogeneous turbulence*

**Video 1**: r-theta cut of density with magnetic field streamlines

**Video 2**: r-phi cut of density with magnetic field streamlines

## Publications

1. A. Vijayan, K. C. Sarkar, B. B. Nath, P. Sharma, Y. Shchekinov, "Extra-planar X-ray emission from disc-wide outflows in spiral galaxies," Monthly Notices of Royal Astronomical Society, in press (arXiv:1801.04282)
2. P. Dhang, P. Sharma, B. Mukhopadhyay, "Magnetized SASI: its mechanism and an explanation for some QPOs in XRBs," Monthly Notices of Royal Astronomical Society, submitted (arXiv:1712.06252)
3. B. Vaidya, D. Prasad, A. Mignone, P. Sharma, L. Rickler, "Scale explicit implementation of anisotropic diffusion with Runge-Kutta-Legendre super-time stepping," Monthly Notices of Royal Astronomical Society, 472, 3147 (2017)

4. D. Prasad, P. Sharma, A. Babul, "AGN jet-driven stochastic cold accretion in cluster cores," Monthly Notices of Royal Astronomical Society, 471, 1531 (2017)
5. N. Yadav, D. Mukherjee, P. Sharma, B. B. Nath, "How multiple supernovae overlap to form superbubbles," Monthly Notices of Royal Astronomical Society, 465, 1720 (2017)

## **Prof. Suryanarayanarao Ramakumar's Lab**

**Team:** Harsh Bansia, Harshavardhan Khare

**Research Areas** (Details below): Crystallography experiments for drug design

**Experimental Setup:** 1056 CPU cores of Cray Sahasrat were used. Parallel version of Amber-CPU package was employed.

### **Performance**

1. 30-40 ns/day in the Cray system compared to 1-2 ns/day in the lab system.

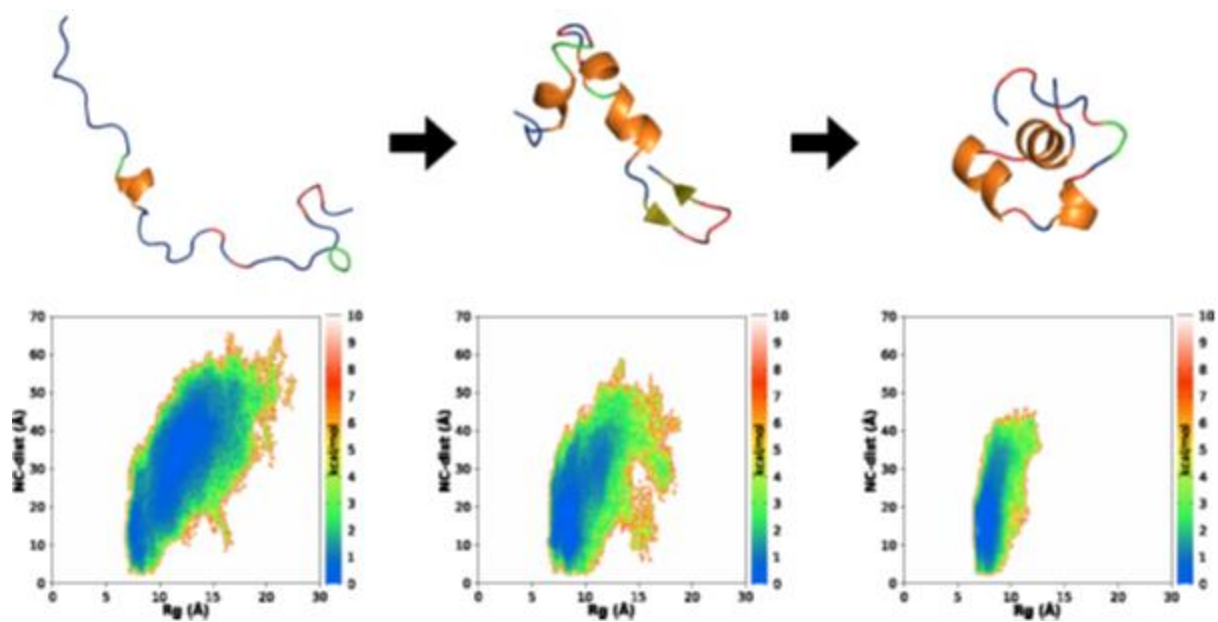
### **Details of Research**

#### **Crystallography Experiments for Drug Design**

Often, protein targets have cryptic pockets which, obscured in unbound protein, become apparent only when ligand is bound and are considered valuable from the perspective of drug design. Through the focused crystallography experiments conducted on the model protein system and subsequent molecular dynamics (MD) simulations, we show that certain glycols act as cryptic pocket finders as they are able to identify a cryptic surface pocket in the protein system studied.

#### **Study of Disordered Proteins**

This research is related to enhanced sampling of conformational ensembles of intrinsically disordered proteins/peptides (IDPs). This involves studying tails of DNA-binding proteins and analysed their properties using various molecular dynamic (MD) methods such as conventional MD temperature-replica exchange MD and accelerated MD. In general this study provides useful insights into the dynamics of important DNA-binding proteins like HU, Ku, Histone-H1 etc which lack unique 3-dimensional structure.



## Publications

1. Certain small glycols as cryptic pocket finders in proteins. Harsh Bansia, Pranjal Mahanta and Suryanarayanarao Ramakumar., *Acta Cryst.* (2017). A73, C263.