Usage of SERC SahasraT Supercomputer for Scientific Applications in IISc in 2020-2021

Supercomputer Education and Research Centre

Indian Institute of Science

Bangalore – 560012

Sourabh S. Diwan

Transition and Turbulence Research Group, Department of Aerospace engineering

Problem statements:

Our group has been using the CRAY system for carrying out direct numerical simulations of transitional and turbulent shear flows, on the following three themes.

1. **Scalar and vorticity transport in turbulent jets**: This involves simulating both steady and transient jets. The former helps in developing a fundamental understanding of the vorticity transport in a jet whereas the latter is applied to computing flows relevant for COVID-19 transmission.

2. **Energy cascade in a turbulent channel flow:** The project aims at studying the turbulent energy cascade from large to small scales by using a bandpass-filter-based multiscale analysis applied to a turbulent channel flow, to enable a better understanding of the mechanism of energy transfer.

3**. Transition in attached and separated flows:** This work involves investigating the intermittency behaviour for the boundary layer transition in attached and separated flows, with applications to MAVs, wind turbine blades etc.

SERC resources: HPC simulations of 1.18million core hours are done on SahasraT in 2020. Data for year 2021 is not available. Requirement of the number of cores in a simulation depends on the nature of work and the queue used. We have used approx. 256 cores in the small queue and 2048-2304 cores in the medium queue.

Parallelization Strategies: Two Incompressible codes are used in our work, both of which are parallelized using MPI. “Megha-V” code is parallelized using the Pencil fast Fourier transform which is incorporated to solve the pressure Poisson equation. The other solver used is an open-source code “Xcompact3d”, which uses the 2DECOMP&FFT library for the same purpose.

Performance: The lab machines are not sufficiently powerful to run these simulations**.**

COVID-19 research using HPC simulations:

Our group has been extensively engaged, over the past two years, in carrying out simulations on the fluid dynamics of respiratory flows such as speech and cough flows with relevance to COVID-19 transmission. The work is being done in collaboration with researchers from NORDITA, Sweden and ICTS-TIFR, Bengaluru.

The first study focuses on the transport of infected aerosol for short-duration face-to-face conversations between two people (lasting up to a couple of minutes), which are typical of the over-the-counter conversations in a supermarket. We find that the risk of infection to a person is much less during a conversation than when they are acting as a passive listener. This is due to the blocking effect of the two speech jets during the conversation, as visualized in figure 1 by an iso-surface of the aerosol. We have carried out a large number of simulations with varying heights of the persons and varying axial separations between the two and mapped the conditions which lead to higher risks of infection. We have also proposed a new method of estimating the probability of infection, which takes into account the viral ingestion through mouth and face, in addition to the inhaled virions.

The second study involves performing simulations on a mild cough flow using an Eulerian treatment for the expelled liquid droplets, which is commonly used in simulating atmospheric clouds. This provides a considerable computational advantage over the Lagrangian methods, which involve tracking of individual droplets. We have compared the performance of our solver with a Lagraingian solver used on a similar problem and found ours to be at least 30 times faster. We have been able to reproduce several known results on cough flows and have obtained new results on the thermodynamics of evaporation. e.g., see figure 2.

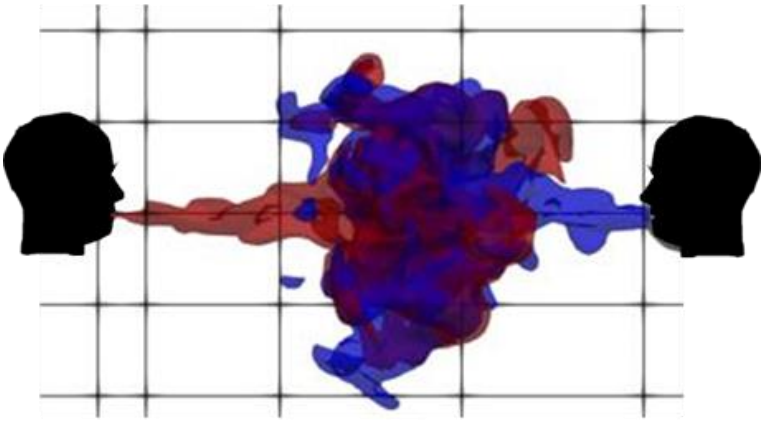


Figure 1. Aerosol cloud generated during conversation between two people of equal height.

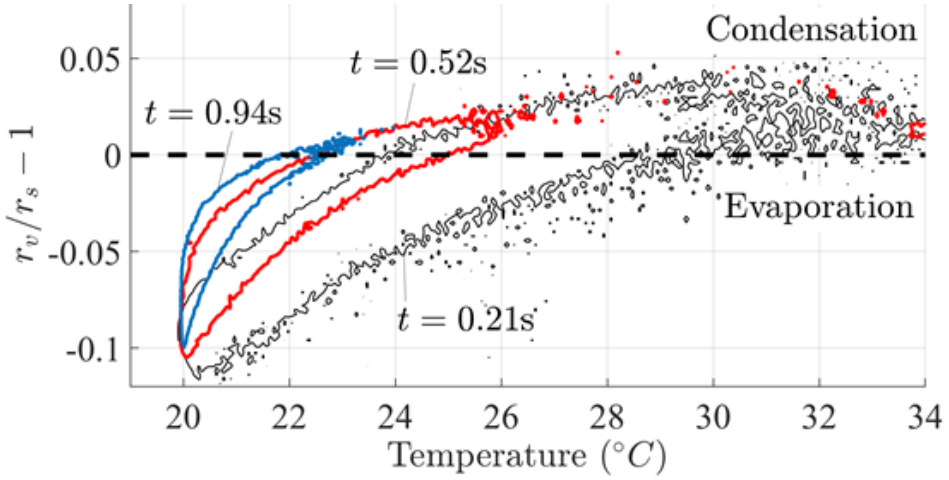


Figure 2. Contours showing evolution of temperature and saturation conditions experienced by droplets in a moist cough. indicates the supersaturation.

Video:

A video on the evolution of the speech flow during conversation between two people of equal height has been sent by email.

Figures on other research themes:

- **Energy cascade in a turbulent channel flow**.

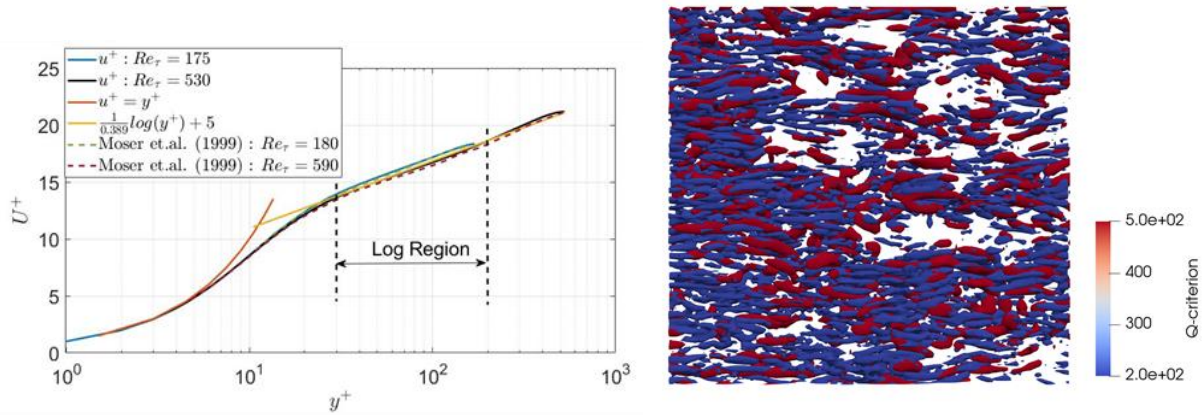


Figure 3 (left): Validation of the mean velocity profiles obtained for the channel flow against those reported in the literature. (right): Iso-surface of the Q-criterion for the velocity field filtered at two scales, i.e. structures of two scales, one of size 10 and other of size 20 (is the local Kolmogorov scale) are shown.

- **Transition in attached and separated flows**

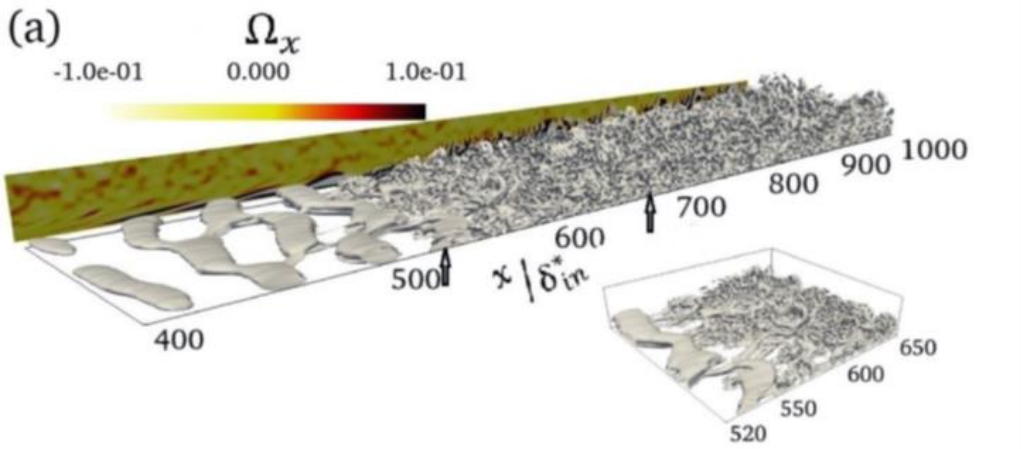


Figure 4. Flow structures indicating the stages in the transition process for a laminar separation bubble. The arrows represent the onset and end of transition respectively.

Publications

Diwan, S. S., Ravichandran, S., Govindarajan, R., & Narasimha, R. (2020). Understanding transmission dynamics of COVID-19-type infections by direct numerical simulations of cough/sneeze flows. *Transactions of the Indian National Academy of Engineering*, *5*(2), 255–261.

Samson, A., Naicker, K., & Diwan, S. S. (2021). Instability mechanisms and intermittency distribution in adverse pressure gradient attached and separated boundary layers. *Physics of Fluids*, *33*(9), 94106.

Singhal, R., Ravichandran, S., & Diwan, S. S. (2021). Direct numerical simulation of a moist cough flow using Eulerian approximation for liquid droplets. *ArXiv Preprint ArXiv:2110.01875*. (Under review for publication)

Singhal, R., Ravichandran, S., Govindarajan, R., & Diwan, S. S. (2021). Virus transmission by aerosol transport during short conversations. *ArXiv Preprint ArXiv:2103.16415*. (Under review for publication)

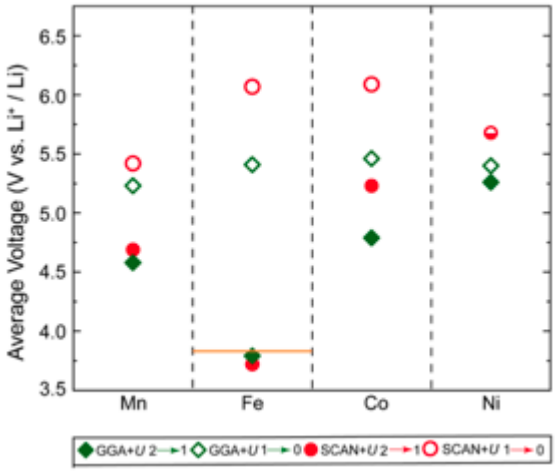
Contribution towards society:

The speech-flow simulations have enabled us to frame public-safety guidelines relevant for short conversations between people. This is particularly relevant in the current times as the society opens up with the risk of asymptomatic COVID-19 infection still present. We plan to share our findings with the public health authorities once our paper is published.

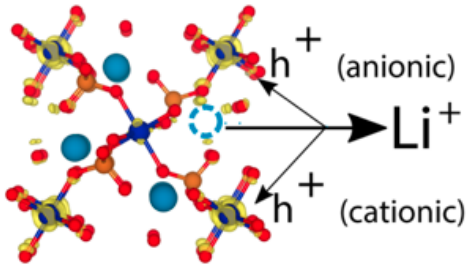
Prof. Prabeer Barpanda (MRC)

Our research effort is focused on beyond the state-of-the-art Lithium-ion batteries. We, in collaboration with Dr. Sai Gautam Gopalakrishnan (Materials Engineering) use SERC facility for computational modeling of battery materials using first principles density functional Theory (DFT) in VASP package. These include the prediction of average intercalation voltage, phase stability, Diffusion co-efficient and the underlying mechanism during the redox processes. Typically, the execution timing for our calculations are 24hours or 72 hours in "small" and "small72" queues.

As calculated average topotactic voltages of monoclinic m-$Li_xMn(SO_4)_2$ (M= Mn, Fe, Co, and Ni).



Redox mechanism



Publications

1. First Principles investigation of anionic redox in bisulfate lithium battery cathodes,
   P. K. Jha, S. Singh, M. Srivastava, P. Barpanda and S. G. Gopalakrishnan.
   Manuscript submitted.
2. First Principles scanning of P-3 type Potassium 3d layered oxide materials for K-ion Battery,
   P. K. Jha, S. N. Totade, P. Barpanda and S. G. Gopalakrishnan.
   In Preparation.

Prof. Chirag Jain (CDS)

HPC resources are crucial for us to develop and benchmark new bioinformatics algorithms for analysis of genome sequencing data. High sequencing throughput, e.g., >1 Tera bp per day from a sequencing instrument requires efficient processing of data to save time and computing costs. Problems of interest in our group include computing mutations in a human genome, de novo genome assembly, and domain specific approximate string pattern matching. We usually focus on either improving the accuracy of analysis, or making the exact solutions run faster by architecture-aware software-design. Our HPC jobs typically run for 24 – 72 hours. They use shared-memory parallelism and parallel disk IO operations. We also require significant storage space on a network attached storage disk to save sequencing data. The figure below is a toy example illustrating *co-linear chaining* of short exact matches (anchors) identified between a pair of DNA sequences. Co-linear chaining is a commonly used module in sequence-analysis tools for approximate matching of two sequences. Our recent work [2] gave an asymptotically faster algorithm for a special case of this problem.

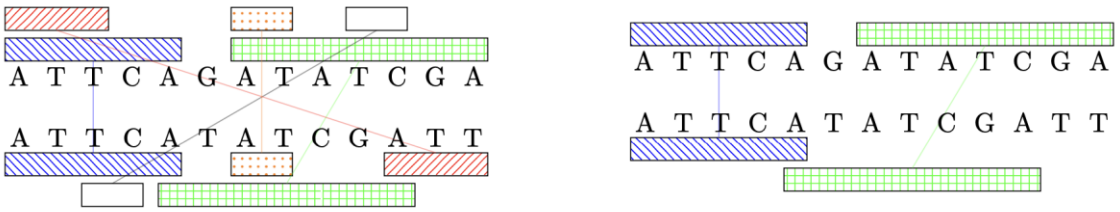


Fig. 1: (Left) Anchors representing a set of exact matches are shown as rectangles. The co-linear chaining problem is to find an optimal ordered subset of anchors subject to some cost function. (Right) A chain of overlapping anchors.

Publications

1. Accelerating minimap2 for long-read sequencing applications on modern CPUs Saurabh Kalikar, Chirag Jain, Vasimuddin Md, Sanchit Misra. Nature Computational Science. (in press)

2. Co-linear chaining with overlaps and gap costs Chirag Jain, Daniel Gibney, Sharma Thankachan. International Conference on Research in Computational Molecular Biology. (accepted)

Jai Sukhatme (CAOS).

1. What science problems did you use SERC machines for?

(1) A fine-scale numerical simulation using an ocean general circulation model of the trapping and homogenization of freshwater during the postmonsoon season in the Bay of Bengal. (2) An investigation using an atmospheric general circulation model of the character of the circulation and transient activity in an atmosphere under uniform boundary forcing but with varying dynamical activity of water vapour. (3) The genesis of mid-tropospheric cyclones over western India and the northeast Arabian Sea using a high-resolution version of the Weather Research and Forecast model. (4) The Analysis and evaluation of the steady-state response of the Asian Monsoon Anticyclone to global warming using an atmospheric general circulation model.

Relevant figures:

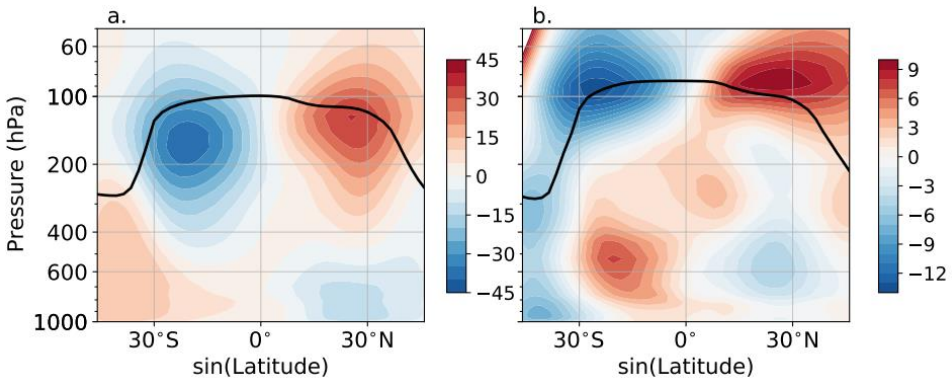


Figure 1. (Item 4) Steady state aquaplanet simulations. Vertical structure of eddy streamfunction (ψ; units: 10^6 m^2 s^{-1}) for (a) warming simulation and (b) difference between warming and control simulations. Note the anticyclone weakens in the upper troposphere while strengthening in the lower stratosphere.

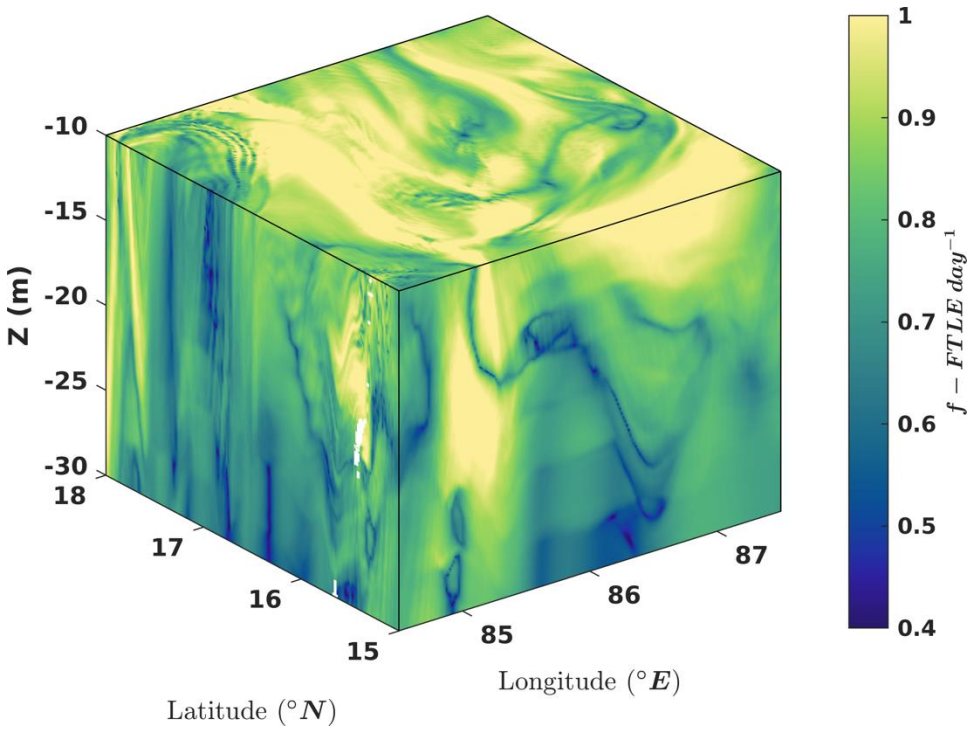


Figure 2: (Item 1) Finite time Lyapunov Exponents calculated from a high-resolution ocean GCM simulation in the Bay of Bengal.

2. Codes or packages used and which machine in SERC did you use. If possible details like number of cores etc.

For Item (4). The simulations were performed on the Cray XC40 (SahasraT) system using 10 nodes and 240 cores. The modules used were: PrgEnv-cray, craype-haswell, cray-mpich, cray-netcdf, cray-parallel-netcdf, cray-libsci, papi, cray-hdf5 and cray-python/3.8.5.0

Related Publications:

1. N. Paul, J. Sukhatme, D. Sengupta and B. Gayen, Eddy induced trapping and homogenization of freshwater in the Bay of Bengal, Journal of Geophysical Research, 10.1029/2021JC017180, 2021.

2. D.L. Suhas, J. Sukhatme and N. Harnik, Dry and Moist Atmospheric Circulation with Uniform Sea-Surface Temperature, Quarterly Journal of the Royal Meteorological Society, 10.1002/qj.4191, 2021.

Santanu Mahapatra (DESE)

Your problem:

The main objective of this work is to gain atomistic insight to non-volatile resistive switching in a monolayer molybdenum disulfide based metal-insulator-metal device. We have used SERC HPC resources to conduct long reactive molecular dynamics simulations using LAMMPS for sulphur vacancy inhabited monolayer MoS_2-based memristor device with inert electrode systems to gain insight into the resistive switching phenomena. We observed that most S atoms residing directly above S vacancies vertically move to the plane of Mo atoms and get stabilized there at a critical applied electric field. The dimension of simulated MoS_2 flake is 18.9 nm × 26.5 nm consisting of about 17160 atoms. To explain both bipolar and unipolar switching operations we have performed MD run of more than 60 ns with different electric fields and electrode materials (graphene/ gold/implicit Lennard-Jones walls).

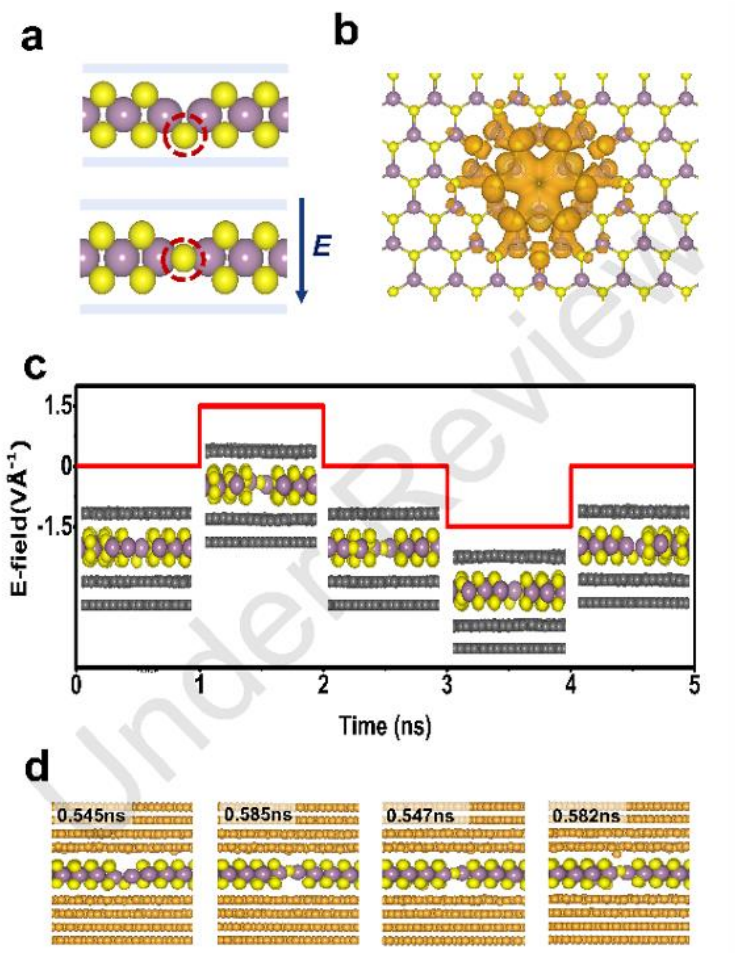


Figure: **a** Zoomed in side-view image showing S atom popping after applying E-field. **b** iso-surface plot after S atom popping at vacancy sites showing metallic states. **c** Snapshots of atomic structures of Graphene-MoS_2-Graphene under different electric-field pulses. **d** Atomic snapshots of Au-MoS_2-Au during different time scales of MD simulations. The external field is applied from the top to the bottom electrode.

SERC's resources

576 CPU cores have been used for each device, i.e., a specific combination of an electrode and MoS_2.

Parallelization strategies

No explicit parallelization strategies are followed as the LAMMPS code is already highly parallel and scalable. However, several benchmarking runs were conducted to determine the limit of the scalability, and it was found that for our specific system, 576 cores are enough for each case. The Kokkos package was used to accelerate the simulations on the CPUs.

Performance

Simulation wall time for 1ns MD run of 17160 atoms is about 7hrs in SERC supercomputer. In our lab, the same simulation takes around 30 hours on a machine with 4 V100 GPUs. Moreover, because of SahasraT, we were able to run multiple simulations and benchmark runs simultaneously which would not have been possible with our lab equipment.

Output

Sanchali Mitra, Arnab Kabiraj and Santanu Mahapatra, “Theory of nonvolatile resistive switching in monolayer molybdenum disulfide with passive electrodes”, *npj 2D Materials and Applications*, 5, 33 (2021)

Vijay Natarajan (CSA)

A Geometry-based Semi-Automated approach to Annotate Data for Polyp Segmentation. The DGX-1 cluster was used to rapidly train our models for polyp segmentation. This application in healthcare was towards the development of AI based methods for assisting doctors in endoscopy procedures.

SERC's resources: DGX-1 cluster. We typically used 2 GPUs in parallel as there were other jobs in the queue. In some instances, we were able to use up to 6 of the 8 GPUs in the cluster

Parallelization strategies employed: We used Tensorflow 1.x with Jupyter notebooks. Out of the box parallelization methods from TensorflowGPU were used.

Performance:

- We found that training runs that took upto 2 days on our local systems (GeForce GTX 1080Ti cards) were completed in 2-3 hours
- However, more time was spent waiting in the queue (5-6 hours) and it was difficult to estimate when the job would be completed.
- We found that it was best to perform a few trial runs on our systems and observe the training progress for a few hours, and scheduling jobs on the DGX cluster. We would cancel the job if there were some issues found.

CoVid 19 research using HPC simulations: N/A

Output:

Publications:

- 1 Patent is under review in the Indian patent office.
- 1 Publication is under preparation for submission to a leading journal in gastroenterology.

Contributions to national/Industry/Societal projects due to the executions, and the resulting impact:

This work has the potential to significantly reduce the data preparation burden in datasets for AI in gastroenterology (and medical datasets in general) Typically, for each training image needs to be prepared by 5 experts, where it takes an expert about 2-3 minutes per image. Hence each image takes a total of 10 minutes of expert time. Preliminary results show that this time can be reduced by 70% to 3 minutes per image (amortized over the entire dataset having around 10k images).

Images and videos: Data from this work cannot yet be released as the work is under peer review and Patent office review.

Attreyee Ghosh (CEaS)

Problem

Our current work focuses on how the Earth's mantle has evolved with time and how that has affected surface features using time dependent models of mantle convection. Starting at a time in the past, we run forward models of mantle convection to address a number of questions about the Earth. One problem we looked into was the interaction of the Indian plate with the Réunion plume that erupted 65 million years ago and how that affected the thickness of the Indian craton. We also looked at the evolution of the Indian Ocean geoid low and what could have caused this negative geoid anomaly over the Indian Ocean to form.

Resources

We used both the SahasraT and the Roddam Narasimha cluster (RNC). Most runs used 96 cores with a maximum of 768.

Parallelization

We use MPI parallelization in a spherical shell geometry.

Performance

Execution times depend on the particular viscosity structure. But a typical run requires 4-5 submissions on SahasraT and 3 submissions on RNC in a 24 hour queue.

Outputs

Publications

1. J. Paul, and A. Ghosh, 2021, Could the Réunion plume have thinned the Indian craton?: Geology, v. 50, p. 346–350, https://doi.org/10.1130/G49492.1.
2. A. Ghosh, D. Pal, 2022, Do lower mantle slabs contribute in generating the Indian Ocean Geoid Low?, Tectonophysics, v. 822, https://doi.org/10.1016/j.tecto.2021.229176.
3. J. Paul, A. Ghosh, 2020, Evolution of cratons through the ages: A time-dependent study, Earth & Planetary Science Letters, v. 531, https://doi.org/10.1016/j.epsl.2019.115962.

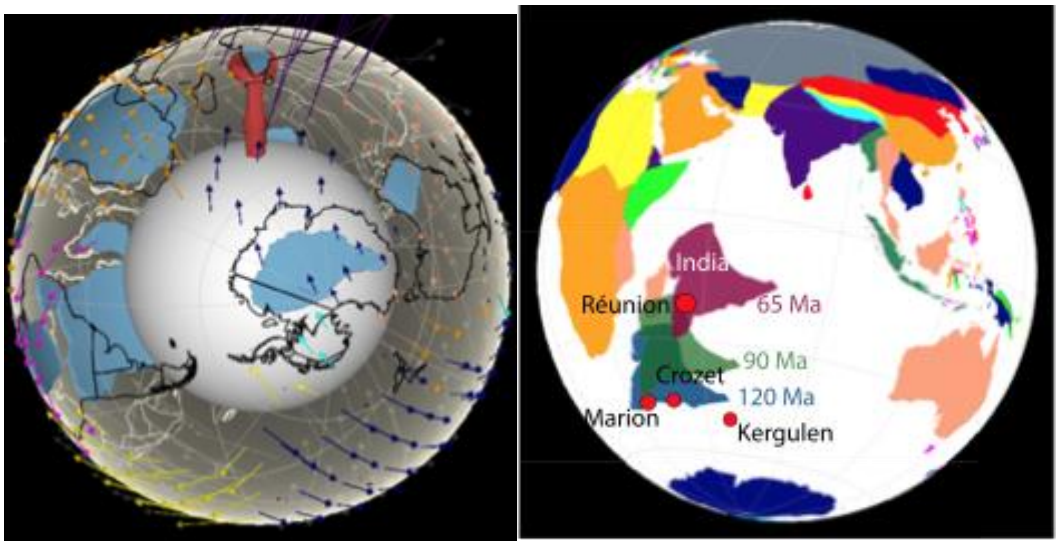
Students Graduated

PhD: Jyotirmoy Paul

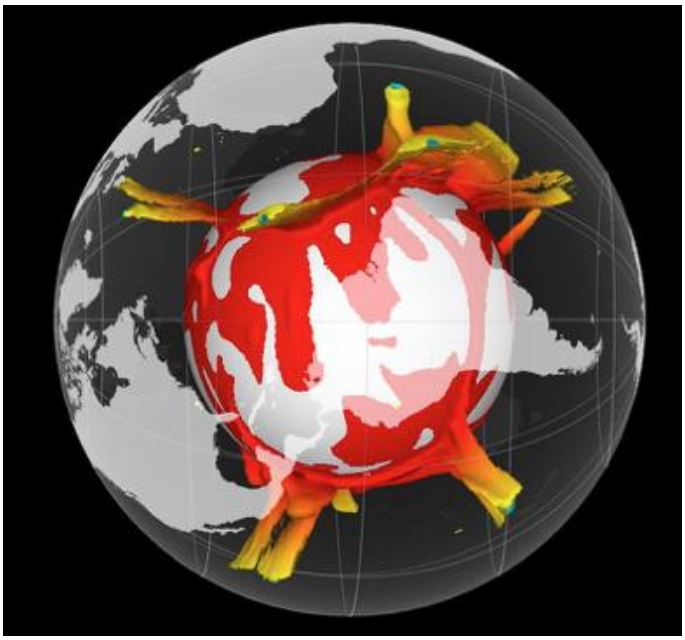
Images and Videos

https://www.youtube.com/watch?v=I3o6LldK5N0&list=UUBruY_7eCEfVjnlriZJGdqw&index=2&ab_channel=GeodynamicsIISc

https://www.youtube.com/watch?v=XvOkgJ6PqGY&list=UUBruY_7eCEfVjnlriZJGdqw&index=8&ab_channel=GeodynamicsIISc



Left: The Réunion plume hitting the Indian plate 65 million years ago. Right: Reconstructed positions of the Indian plate from 120 million years ago till the present day along with reconstructed plumes and their eruption ages (Paul & Ghosh, 2021).



Temperature isosurfaces from one of our time-dependent models. Red indicates hot upwellings emerging from the core-mantle boundary and reaching the surface of the Earth.

Prof. Ananth Govind Rajan (Chemical Engineering)

Problems solved: We used SERC resources to carry out classical molecular dynamics (MD) simulations as well as quantum-mechanical density functional theory (DFT) calculations of nanomaterial systems. These simulations were aimed at understanding the controlled synthesis of nanoporous two-dimensional (2D) materials, as well as their use in seawater desalination applications. We also determined the reaction mechanisms of electrocatalytic processes, such as electrochemical CO_2 reduction and water splitting, using DFT calculations.

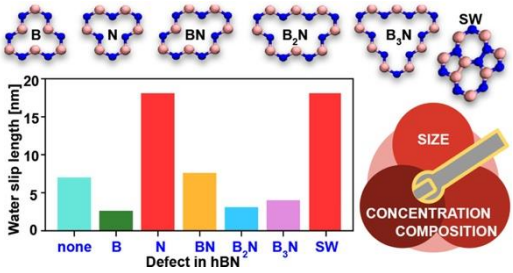
SERC resources used: We used the SahasraT (Cray XC40) supercomputer at SERC to carry out our simulations and calculations.

Parallelization strategies employed: DFT calculations were carried out using 96 cores of computing power and MD simulations using 48 cores of computing power. The codes employed, such as the large-scale atomic/molecular massively parallel simulator (LAMMPS) for MD simulations and the Vienna ab initio simulation package (VASP) for DFT calculations support parallelization over multiple cores.

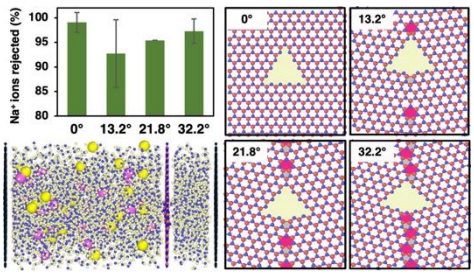
Performance: Typical execution time on SahasraT for the DFT calculations ranged from 48 to 96 hours and that for MD simulations ranged from 24 to 48 hours. It would not be possible to do these calculations and simulations on a simple workstation.

Publications:

- Seal, A., **Govind Rajan, A.*** Modulating Water Slip Using Atomic-Scale Defects: Friction on Realistic Hexagonal Boron Nitride Surfaces. *Nano Lett.* **2021**, 21 (19), pp 8008–8016.



- Sharma, B. B., **Govind Rajan, A.*** How Grain Boundaries and Interfacial Electrostatic Interactions Modulate Water Desalination Via Nanoporous Hexagonal Boron Nitride. *J. Phys. Chem. B*, Article ASAP, DOI: 10.1021/acs.jpcb.1c09287.



Rajesh Sundaresan (ECE and RBCCPS)

Problem description: We built city-scale agent-based epidemic simulators to model COVID-19 spread in Bengaluru and Mumbai, each with roughly 12.4 million agents. The simulators were used to study the impact of various targeted interventions like case isolations, home quarantines, ward containments, lockdowns, etc. We also used the simulators to study various unlock scenarios. Further, we also used the simulators to understand the impact of opening public transport on the pandemic in Mumbai, particularly the Mumbai locals.

SERC resources used: We used the Sahasra T platform. I believe we used at peak usage about 12 cores/node and about 20 nodes. We used 172734.76 CPU core hours on the Sahasra T.

Parallelisation strategies employed: We attempted to parallelise the implementation using the Open MPI framework but were not successful. Eventually, we simply ran different instances in different cores and combined the results using scripts.

Performance: The execution times were not too different. But we exploited the capability to launch parallel runs.

CoVid 19 research using HPC simulations: Our work was in response to the pandemic. We built city-scale agent-based epidemic simulators to model COVID-19 spread in Bengaluru and Mumbai, each with roughly 12.4 million agents. The simulators were used to study the impact of various targeted interventions like case isolations, home quarantines, ward containments, lockdowns, etc. We also used the simulators to study various unlock scenarios. Further, we also used the simulators to understand the impact of opening public transport on the pandemic in Mumbai, particularly the Mumbai locals.

Publications:

- S.Agrawal et al., City-scale agent-based simulators for the study of non-pharmaceutical interventions in the context of the COVID-19 epidemic, Journal of the Indian Institute of Science, vol. 100, pp. 809-847, November 2020
- A. Talekar, et al., Cohorting to isolate asymptomatic spreaders: An agent-based simulation study on the Mumbai Suburban Railway. The 20th International Conference on Autonomous Agents and Multiagent Systems, AAMAS-2021, May 2021. Full version.

Contributions to the national/Industry/societal projects due to the executions, and the resulting impact: We shared our findings with the Karnataka Disaster Management Authority. Our TIFR Mumbai colleagues shared their findings with the Brihanmumbai Municipal Corporation. Our scenario projections were helpful inputs to various stakeholders as the unlock unfolded.

Images and videos:

- Mumbai simulation outcome (jpg file)
- Link to Bengaluru and Mumbai city populations across wards (jpg file)
- Cohorting strategies for targeted isolation of asymptomatic spreaders of COVID-19 (1.5 min link to YouTube video)

1. **Department of Materials Engineering (ME) Prof. Praveen C. Ramamurthy's Lab**

Research

Two-dimensional (2D) materials beyond graphene constitute a 2D flatland, which has become one of the active and emerging current research field. As 2D layers are held together by a van der Waals (vdW) force, the realization of vertical structures based on these layers is an approach that offers a rich platform to study fascinating vdW force-driven properties, like, commensurate lattice coincidence, electronic structure and band structure, magnetic and transport properties, spin-orbit coupling, or exchange coupling induced by proximity effect and inversion symmetry breaking. In this aspect, the integration of intrinsic 2D ferromagnets with vdW semiconductors will become fertile ground for fundamental science as well as of great practical interest toward the seamless integration of electron transport. In this framework, we plan to perform systematic first principles investigations on magnetic proximity effects induced within the 2D ferromagnetic layer-vdW heterostructures. The primary focus will be on elucidating the impact of magnetically doped and intrinsic 2D ferromagnets on the electronic structure and quantum transport properties of such systems with stable and large valley and spin polarization. Moreover, channel transport in nanoscale and spectral function projection techniques will be performed using large supercell calculations to reconstruct the primitive-cell band structure to determine the electron device functionality (i.e., photovoltaic/sensors) of the heterostructure system with an expectation of experimental realization. All the simulation will be performed using an appropriate *ab initio* simulation platform.

SERC Resources and Experiments

Up to 4 GPU cores of the NVIDIA-DGX GPU cluster. In most of the problems, the commonly used HPC resources are debug, small and small72 queue with 40 cores. However, in a few cases, we have also utilized medium queue. A parallel code Quantum Espresso, WannierTools were used, with both multicore and multinode parallelization.

Parallelization

GPU version of the simulation platform.

Performance

The execution on normal CPU based systems would run for around a month and a half, but it would complete within a week on the NVIDIA-DGX machine. The computational facilities at SERC are much faster than our lab server facility. 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 lab facility.

CoVid 19 research using HPC simulations

Not Applicable

Outputs:

Three manuscripts under preparation.

Dr. Sai Gautam Gopalakrishnan's lab (Department of Materials Engineering)

Research:

Our group uses the SERC-HPC facility to perform ab-initio computations to design and discover materials for energy storage (beyond Li-ion systems) and energy harvesting (photovoltaics and thermochemical water-splitting) applications. The HPC resources were extensively used to perform first-principles density functional theory (DFT) calculations to address several computationally intensive problems pertaining to defect energetics, thermodynamic, kinetic, electronic, and structural properties of materials. The HPC support was also used to generate datasets aiding machine learning prediction models. Important projects include:

- Assessing several exchange-correlation functionals' accuracy and computational performance in predicting migration barriers in candidate electrode and electrolyte materials.
- Performing high-throughput calculations to explore candidate cathode materials for calcium ion batteries and studying the thermodynamic stability of iron fluoride-based cathode materials for sodium, potassium, and ammonium-ion batteries.
- First-principles investigation of anionic redox in bisulphate lithium-ion battery cathodes.

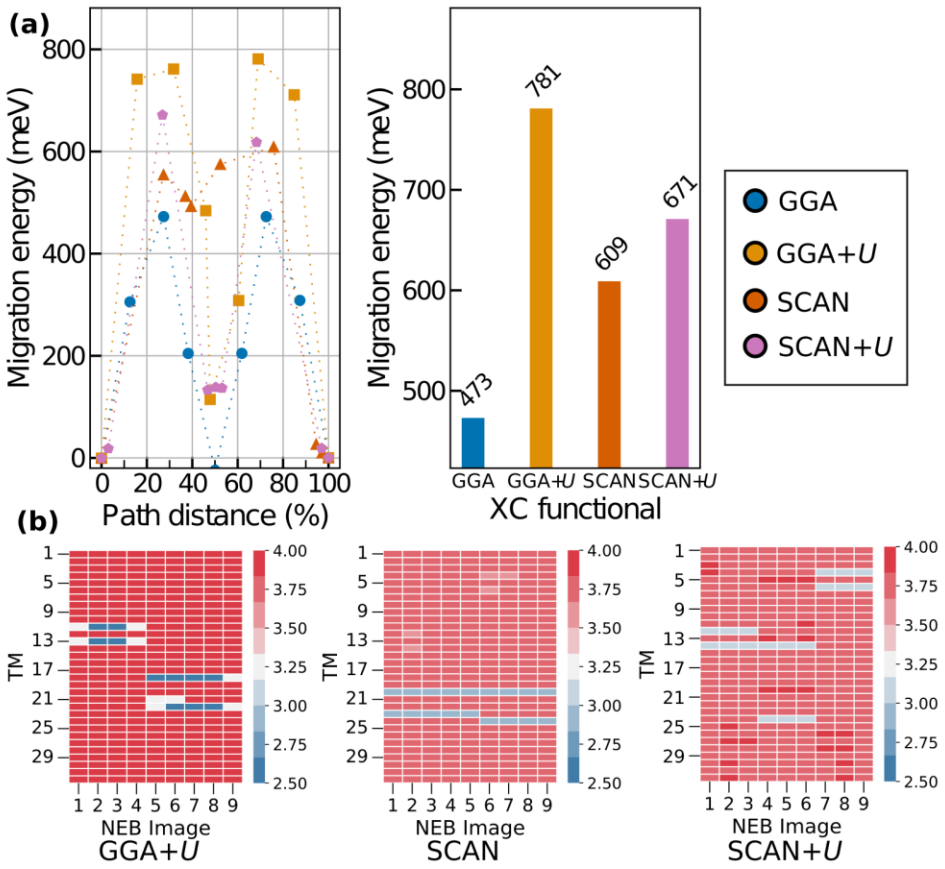


Figure:(a) Migration barriers and the corresponding minimum energy paths computed for $MgMn_2O_4$ spinel for different exchange-correlation functionals by performing nudged elastic band calculations (NEB). (b) On-site magnetic moment changes for the transition metal (Mn) in the $MgMn_2O_4$ structure as a function of image numbers (i.e., as Mg is undergoing migration), where 1stand 9th images correspond to the initial and final Mg sites, respectively

SERC's Resources:

Our lab used the CRAY XC40-SahasraT HPC system with core counts ranging from 1 to 2400 and wall time varying between 24 to 72 hours.

Parallelization Strategies:

All calculations were performed using VASP (Vienna Ab initio Simulation Package), which uses the Intel-MPI parallelization libraries.

Performance:

Our lab cluster has a comparatively lesser number of cores (4 nodes of 128 cores each) but enables high wall time (168 hours) and lesser cluster wait time when compared to the SahasraT HPC system. Typical wait time for jobs demanding higher resources varies between 1-4 weeks on the CRAY XC40 machine. SahasraT HPC system offers faster execution when compared to the local facility especially for jobs involving high computational resources.

Students Trained:

One IISC-UG student completed his BS thesis and will soon submit his MS thesis. Three Ph.D. and two MTech students continue utilizing the SERC services for their research. One postdoctoral fellow currently avails the SERC-HPC facility.

Contributions:

The underlying objective behind the projects executed is to identify candidate materials for battery and photovoltaic applications, which plays a crucial role in establishing low-carbon economy.

Publications:

1. P. Kr. Jha, S. Singh, M. Srivastava, P. Barpanda and Gopalakrishnan Sai Gautam, First-Principles Investigation of anionic redox in bisulfate lithium battery cathodes. (Manuscript submitted)
2. P. Kr. Jha, S. N. Totade, P. Barpanda and Gopalakrishnan Sai Gautam, First-Principles scanning of P-3 type Potassium 3d layered oxide materials for K-ion Battery. (In preparation)
3. Reshma Devi, Baltej Singh, Pieremanuele Canepa, and Gopalakrishnan Sai Gautam, Effect of Exchange-Correlation Functionals on the Estimation of Migration Barriers in Battery Materials. (Manuscript Submitted)
4. Ankit Kumar, Dereje Bekele Tekliye, Xie Weihang, Thelakkattil Devassia Mercy, Pieremanuele Canepa, Gopalakrishnan Sai Gautam, Exploration of NaSICON frameworks as calcium-ion battery cathodes. (In preparation)

Manish Jain (Physics)

Research: Two-dimensional materials offer unprecedented control over a large variety of properties that can potentially be engineered on-demand. This creates exciting prospects for applications of these materials in a wide variety of fields. Some twisted bilayers have tantalizingly similar phase diagrams as high-T_c superconductors. Also, twisted multilayer systems, which can be experimentally routinely made, have a large phase space of choice of materials and twist angles, with fascinating properties hidden in this phase space. Our group has been interested in understanding and calculating properties of twisted bilayers of two-dimensional materials.

SERC resources used: We used the SahasraT (Cray XC40) supercomputer at SERC to carry out our calculations. Our calculations typically would use the medium and large queue on the machine with 200 to 400 nodes (4800 to 9600 CPU cores)

Parallelization strategies employed: Density Functional Theory (DFT) calculations were carried out using SIESTA as well as Quantum Espresso packages. These *ab initio* DFT packages scale to 1000's of cores and have been used to solve these difficult problems involving up to 27,000 atoms. Such calculations are state-of-the-art and among the largest calculations done with these packages to date. We also combine the DFT calculations with molecular dynamics simulations using LAMMPS (for relaxation of structures).

Performance: Typical execution time on SahasraT for the DFT calculations ranged from 8 to 96 hours, and that for MD simulations ranged from 10 to 48 hours. It would not be possible to do these calculations and simulations on any other machine available to us.

Students Trained: Five Ph.D. students utilize the SERC services for their research. Without this facility they would simply not be able to work on the problems we have chosen to work on. One PhD student, Indrajit Maity, graduated in 2021.

Contributions: The underlying objective is to study fundamental issues associated with electronic structure, dynamical and optical properties of twisted two-dimensional materials.

Publications:

1. Kimberly Hsieh, Vidya Kochat, Tathagata Biswas, Chandra Sekhar Tiwary, Abhishek Mishra, Gopalakrishnan Ramalingam, Aditya Jayaraman, Kamanio Chattopadhyay, Srinivasan Raghavan, Manish Jain, and Arindam Ghosh, Spontaneous Time-Reversal Symmetry Breaking at Individual Grain Boundaries in Graphene, Physical Review Letters 126, 206803 (2021).
2. Indrajit Maity, Prabal K. Maiti, H. R. Krishnamurthy, and Manish Jain, Reconstruction of moiré lattices in twisted transition metal dichalcogenide bilayers, Physical Review B 103, L121102 (2021).
3. Shashank Kumar Ojha, Sanat Kumar Gogoi, Prithwijit Mandal, S. D. Kaushik, J. W. Freeland, M. Jain, and S. Middey, Oxygen vacancy induced electronic structure modification of KTaO3, Physical Review B 103, 085120 (2021).
4. Shaili Sett, Sudipta Kundu, Saloni Kakkar, Navkiranjot Kaur Gill, Manish Jain, Arindam Ghosh, Anomalous electrical transport in orientationally controlled trinary hybrids of graphene and twisted bilayer molybdenum disulphide, Bulletin of Materials Science 44, 1 (2021).

Prof. Abhik Choudhury(Materials Engineering)

Research: Microstructure evolution modelling during phase transformations typically results in spontaneous pattern formation that are important for the physics and materials communities. Our research in the years 2020-2021 has been focussed on the modelling and simulation of microstructural evolution during multicomponent multi-phase phase transformation. Specifically, the focus of the research has been to unravel the influence of solid-solid and solid-liquid interfacial energy anisotropy on the formation of microstructures during eutectic reactions. Additionally, studies of microstructural evolution during spinodal decomposition of ternary organic photovoltaic blends that have implications for the fabrication of photo-voltaic cells have been undertaken. A virtual framework in the spirit of ICME(Integrated Computational Materials Engineering) allowing for the determination of process-structure and structure-property correlations was formulated that enabled the optimization of fabrication processes and blend compositions delivering the maximum photovoltaic efficiency.

SERC resources used: We used the SahasraT (Cray XC40) supercomputer at SERC to carry out our calculations. Our calculations typically would use the medium and large queue on the machine. Our runs usually utilized from Us for the different simulations conducted during the last two years.

Parallelization strategies employed: Our codes are parallelized using MPI employing 3D and 2D domain decomposition strategies allowing for massive parallelization. We adopted parallel file writing strategies based on hdf5 libraries that enabled efficient input-output operations.

Performance: The resources available as part of SahasratT allowed us to investigate microstructure evolution in 3D dimensions for a large number of material parameter variations which would have been impossible on the clusters on our systems. While the largest simulations utilized about a million CPU core hours, typical simulation runs on smaller systems required 48—72 hours for completion.

Students trained: Two Phd students, two master students and two UG students have utilized the resources for their research work in the last two years.

Contributions: Establishing the influence of anisotropy in the solid-solid interfacial energy on microstructure evolution during bulk binary and ternary; two-phase and three-phase growth. Formulation of a virtual framework for the optimization of photo-voltaic cell fabrication.

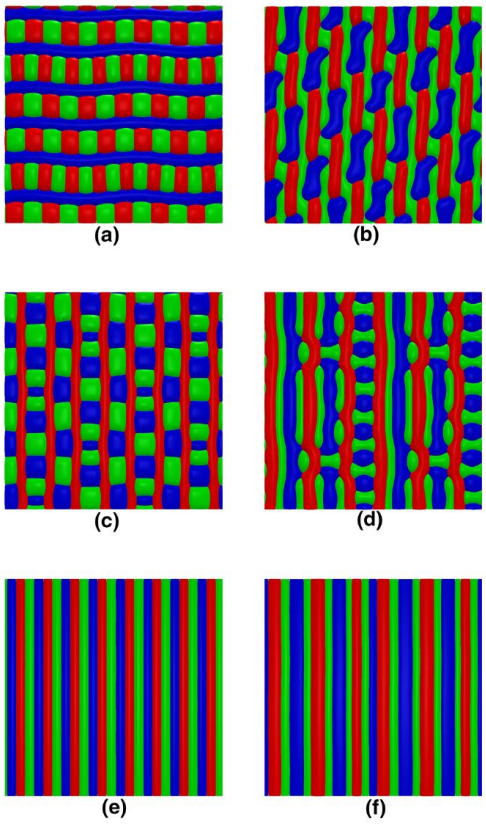


Fig. 21—Steady state solid-liquid interface contour for the extended simulations. Left column is for $D^l = (1, 1)$ and the right column is $D^l = (2, 1)$. (*a*, *b*) Only $\alpha - \beta$ is anisotropic; (*c*, *d*) $\alpha - \beta$ and $\alpha - \delta$ are anisotropic; ((*e*, *f*) All three interfaces $\alpha - \beta$, $\alpha - \delta$ and $\beta - \delta$ are anisotropic. All images are tiled 2×2. The red, green and blue colors depict the α, β and δ phases respectively (Color figure online).

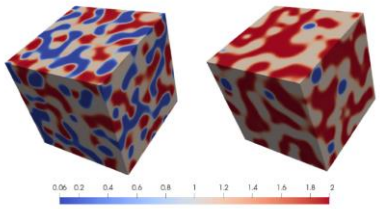


FIG. 8. Morphology of device exhibiting the highest efficiency (blend composition: 0.32:0.34:0.34) on the left and the lowest efficiency (blend composition: 0.04:0.45:0.51) on the right for the DAA system. On the color bar, 0 corresponds to the polymer rich phase, 1 corresponds to the fullerene rich phase, and 2 corresponds to the ternary component rich phase.

Publications:

1. S. Khanna, S. K. Aramanda, A. Choudhury; *Role of Solid–Solid Interfacial Energy Anisotropy in the Formation of Broken Lamellar Structures in Eutectic Systems, Metallurgical and Materials Transactions A*; 51 6327-6345 (2020)
2. S. K. Aramanda, S. Khanna, S. K. Salapaka, K. Chattopadhyay, A. Choudhury, *Crystallographic and Morphological Evidence of Solid–Solid Interfacial Energy Anisotropy in the Sn-Zn Eutectic System; Metallurgical and Materials Transactions A,* 51 6387–6405 (2020)
3. Khanna, S., Choudhury, A.; *Three-Phase Eutectic Microstructures: Influence of Interfacial Energy Anisotropy and Solute Diffusivities; Metallurgical and Materials Transactions A, 52 4246—4263 (2021)*
4. Khanna, S., Choudhury, A.; *Role of interfacial energy and liquid diffusivities on pattern formation during thin-film three-phase eutectic growth; Journal of Materials Science, 56 17646—17664 (2021)*

5. Fiyanshu Kaka, Sumeet Khanna, P.C.Ramamurthy, Abhik Choudhury; Investigation of process-structure–property relationship in ternary organic photovoltaics, *Journal of Applied physics, 128, 145501(2020)* (Selected as a featured article; an image from the paper was selected as a cover page of the issue)

Prof. K. Kesava Rao (retired, Chemical Engineering)

Problem statement: We are studying the flow of granular materials through vertical channels of rectangular cross section and circular pipes. To obtain an insight in the rheology, the particle dynamics computer simulations, also well known as the Discrete Element Method (DEM), are performed using SERC's HPC resources. Different continuum models are tested and compared with the results of the DEM and experiments. When the bulk solids fraction phibar, the ratio of the volume of the solids to the volume of the channel is varied, a steady flow is observed for higher values of phibar. An oscillatory state and then an accelerated flow occurs as phibar decreases below a critical and a minimum value, respectively. In steady fully developed flow, different regimes having distinct rheological properties are observed. Some of these features are intriguing; these motivate researchers to pursue better continuum models for granular flow. This is a joint work with my Ph. D student Mr. Bhanjan Debnath and Prof. V. Kumaran.

SERC's resources: The simulations are performed in SahasraT using 120 to 480 CPU cores.

Parallelization: We used the LAMMPS packages to run the simulations.

Performance: For the range 0.1 - 0.5 million particles, one simulation takes 18 - 22 hours using 240 cores, whereas it takes more than 72 hours using 480 cores with more than 2.5 million particles. These simulations are highly time-consuming. Running these simulations in lab workstations with 4 - 16 cores may take more than a week.

Publications:

1. Debnath B, V Kumaran, **Kesava Rao K**. Comparison of the compressible μ(I) class of models and non-local models with discrete element method (DEM) for steady fully developed flow of cohesionless granular materials through a vertical channel. *J. Fluid Mech.,* 2022 (accepted, in press)
2. Debnath B, **Kesava Rao K**, V Kumaran. Different shear regimes in the dense granular flow in a vertical channel. (Under review)

Prof. V Kumaran (Chemical Engineering)

Problems solved: We are currently working on the turbulent flow statistics of rarefied gases at high Mach numbers using the Direct Simulation Monte Carlo method. In this regard, we used SERC resources to perform simulations using our in-house developed code and the open-source software namely Stochastic Parallel Rarefied-gas Time-Accurate Analyzer (SPARTA). This study is aimed at understanding the channel flow behaviour, near wall effects, energy spectrum and dissipation spectrum at hypersonic flow conditions.

SERC resources used: We used the SahasraT (Cray XC40) supercomputer at SERC to perform numerical simulations.

Parallelization strategies employed: We have employed Message Passing Interface (MPI) parallelization for our in-house code and the software we used: SPARTA was also developed using MPI. To this extent, we used around 1000 processors for both cases.

Performance: The execution time on the Sahasra T cluster was around 10 to 24 hours. It would have taken days on a local cluster or on a personal computer.

Publications: The work is still in progress.

Prof. G. Bala's research Group (CAOS):

Problems solved using SERC resources in 2020 and 2021:

Effects of local and remote black carbon aerosols on Indian Monsoon: we performed idealized climate model simulations to assess the relative impacts of an increase in local black carbon (BC) aerosols (located over the Indian region) and the remote BC aerosols (located outside the Indian region) on the summer monsoon precipitation over India.

Stratospheric aerosol geoengineering to counter climate change: We performed idealized climate model simulation to investigate the effect of a specific microphysical property of sulfate aerosols in the stratosphere: hygroscopic growth—the tendency of particles to grow by accumulating water.

SERC's resources: Several climate model simulations were run on CRAY XC40 SahasraT. Each simulation used 240 cores for 144 wall-clock hours.

Publications (2020-2021) using SERC computing resources:

1. Krishnamohan, KS, Angshuman Modak, **G. Bala,** 2021: Effects of local and remote black carbon aerosols on summer monsoon precipitation over India, Environmental Research Communications, https://doi.org/10.1088/2515-7620/ac18d1
2. Tresa Mary Thomas, **G. Bala** and V. V. Srinivas, 2021: Characteristics of the Monsoon Low Pressure Systems in the Indian Subcontinent and the Associated Extreme Precipitation Events, Climate Dynamics, https://doi.org/10.1007/s00382-020-05562-2
3. Thejna Tharammal, **G. Bala**, André Paul, David Noone, Astrid Contreras-Rosales, Kaustubh Thirumalai, 2020: Evolution of Asian monsoon and stable water isotope ratios during the Holocene: Isotope-enabled climate model simulations and proxy data comparisons, Quaternary Science Reviews, https://doi.org/10.1016/j.quascirev.2020.106743
4. Krishnamohan, KS, **G. Bala**, Long Cao, Lei Duan and Ken Caldiera, 2020: The climatic effects of hygroscopic growth of sulfate aerosols in the stratosphere, Earth's Future, **https://doi.org/10.1029/2019EF001326**

Image from our study on the effects of black carbon aerosols on the Indian summer monsoon rainfall:

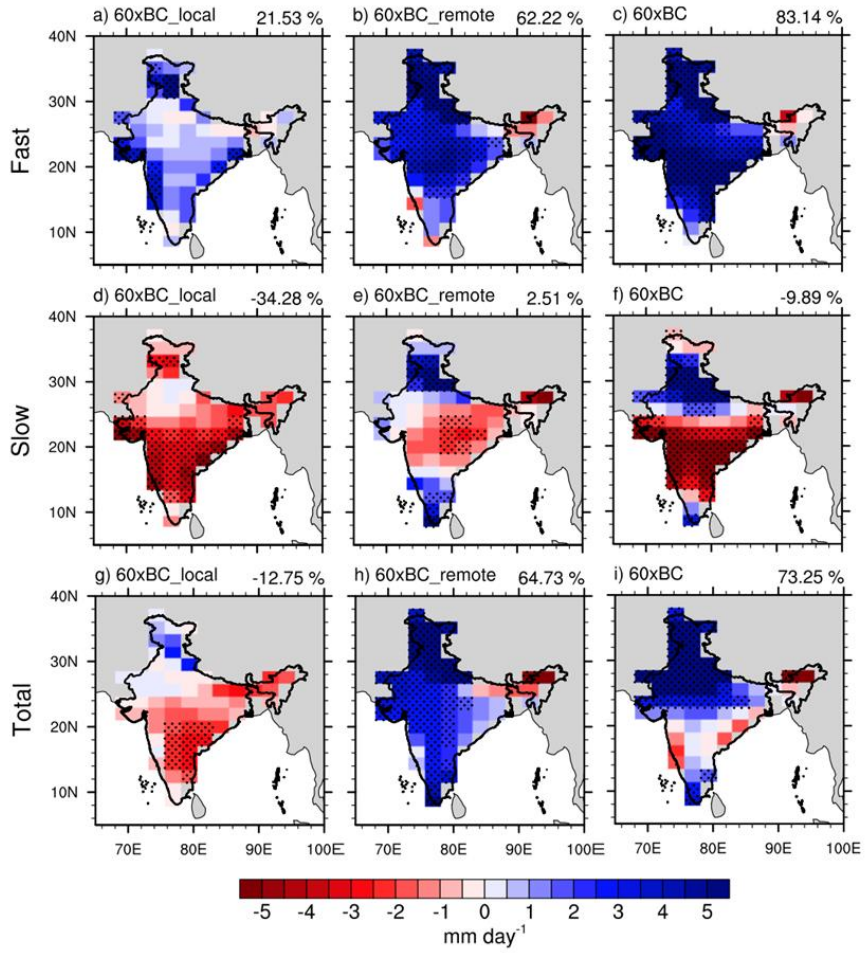


Figure Caption: The contribution to the change in June-September (JJAS) mean precipitation (mm/day) over India by fast adjustments (top panels), slow response (middle panels) and the total change (bottom panels) in the 60xBC_local (left panels), 60xBC_remote (center panels) and 60xBC (right panels) experiments relative to the 1xBC simulation. Fast adjustment refers to the changes related to black carbon aerosol forcing, slow response refers to the change that scales with the surface mean temperature change, and total change is the sum of fast adjustment and the slow response. The mean changes (in percentage) over India are shown in the top right corner of each panel. The stippling in the panels indicates the regions where the changes are larger than two standard deviations (confidence level of about 95%) estimated from 20 JJAS means of the 1xBC prescribed-sea surface temperature simulation for the fast adjustments, and 50 JJAS means of the 1xBC slab ocean simulation for the slow response and total response.

Dr. Phani Motamarri 's Lab (CDS):

Problem Statement:

Develop finite-element based scalable computational methodologies (DFT-FE) on hybrid CPU-GPU architectures for accelerating quantum-mechanical simulations at extreme-scale using density functional theory and leverage these techniques to address complex materials problems not accessible before. One of our research projects involves developing computational methods to understand Li dendritic growth in solid-state electrolytes in the presence of an electric field. As a first step, an ab-initio molecular dynamics framework with various thermostats to calculate transport properties and nudged elastic band to calculate transition state activation energy were implemented in the open-source code DFT-FE and tested for accuracy and performance. To this end, properties like formation energy, diffusivity, and Li migration barrier of solid electrolyte materials were benchmarked with state-of-the-art plane-wave based codes like quantum espresso using HPC resources at SERC.

SERC Resources:

We used SahasraT (Cray XC40) supercomputer at SERC to calculate the formation energy, activation energy and diffusivity from Quantum Espresso. Formation energy calculations for DFT-FE were also done on SahasraT. The core-hour utilization in 2021 was 17,00,000. The number of CPU cores used was anywhere from 200 cores to 4000 cores on SahasraT .

Parallelization:

DFT-FE is a massively parallel finite-element based DFT solver that employs MPI. DFT-FE employs 3 levels of parallelization: a) domain decomposition b) k-point parallelization c) band parallelization.

Performance:

In-house cluster is 2 nodes with 16 GPUs is mainly for quick testing of in-house algorithmic implementations but running long node-hr jobs required for ab-initio Molecular dynamics simulations is not feasible.

Output:

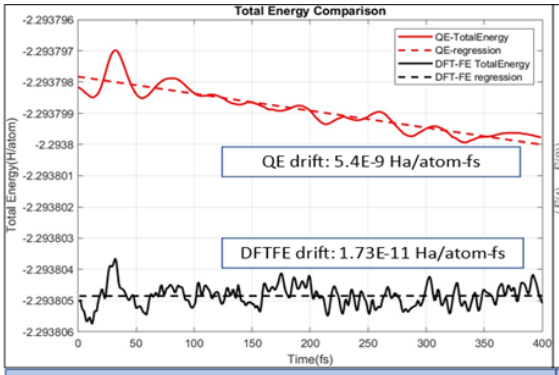


Fig: 1 Comparison of Energy drift of Quantum Espresso(NVE) and DFT-FE(NVE).

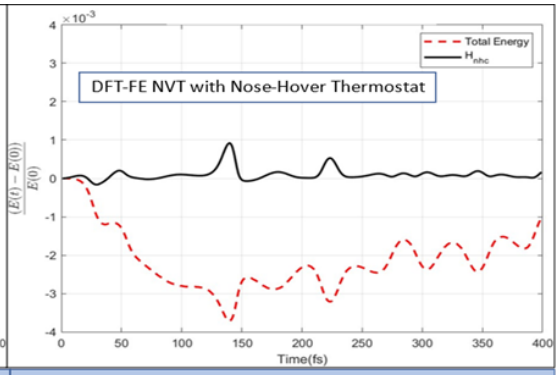


Fig: 2 Conservation of H_{nhc}(Nose-Hover Chains Hamiltonian) in DFT-FE MD NVT.

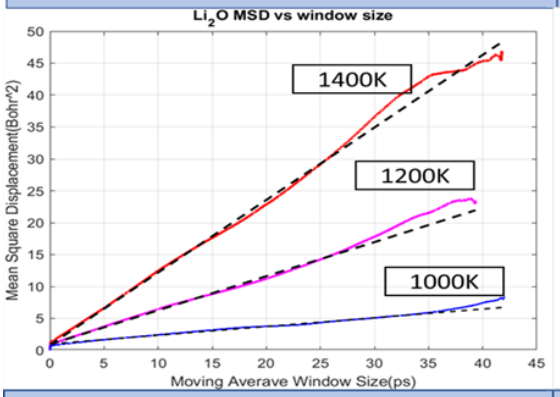


Fig:3 Diffusivity of Li vacancy in Li_2O

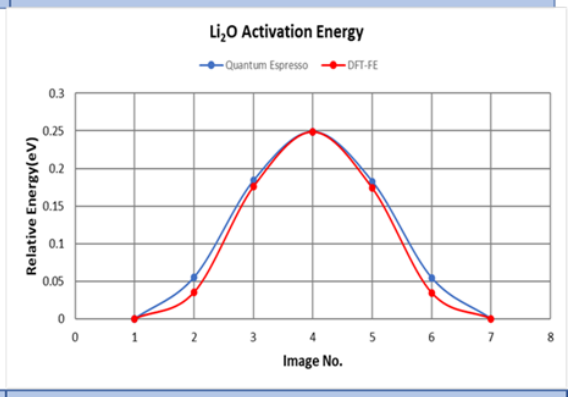


Fig: 4 Activation Energy for Li hop in Li_2O

Publications:

1. Kartick Ramakrishnan, Sai Gautam Gopalakrishnan, Phani Motamarri*: An ab-initio benchmarking study of solid electrolyte material properties using finite-element discretization of DFT (DFT-FE) (under preparation)
2. Gourab Panigrahi, Debashis Panda, Phani Motamarri*: "A matrix-free computational framework for finite-element discretized matrix multi-vector multiplication on hybrid CPU-GPU architectures" (under preparation)
3. Kartick Ramakrishnan, Sai Krishna Kishore Nori, Phani Motamarri*, Satadeep Bhattacharjee, Seung-Cheol Lee, Gour P Das: Projected Finite-element Orbital Population Analysis: A robust approach for extraction of chemical bonding information from large-scale DFT calculations (submitted):
4. Sambit Das, Phani Motamarri, Vishal Subramanian, David M Rogers, Vikram Gavini: DFT-FE 1.0— Algorithmic and implementation innovations for massively parallel finite-element based Kohn-Sham DFT calculations on hybrid CPU-GPU architectures (submitted)

Prof. Ratnesh K. Shukla (Mechanical Engineering)

Problem Statement

We have used SERC resources for the computation of compressible multiphase flows with higher-order methods. These flows contain shocks, material-interfaces and several small-scale features resolution of which is computationally challenging

SERC's resources used

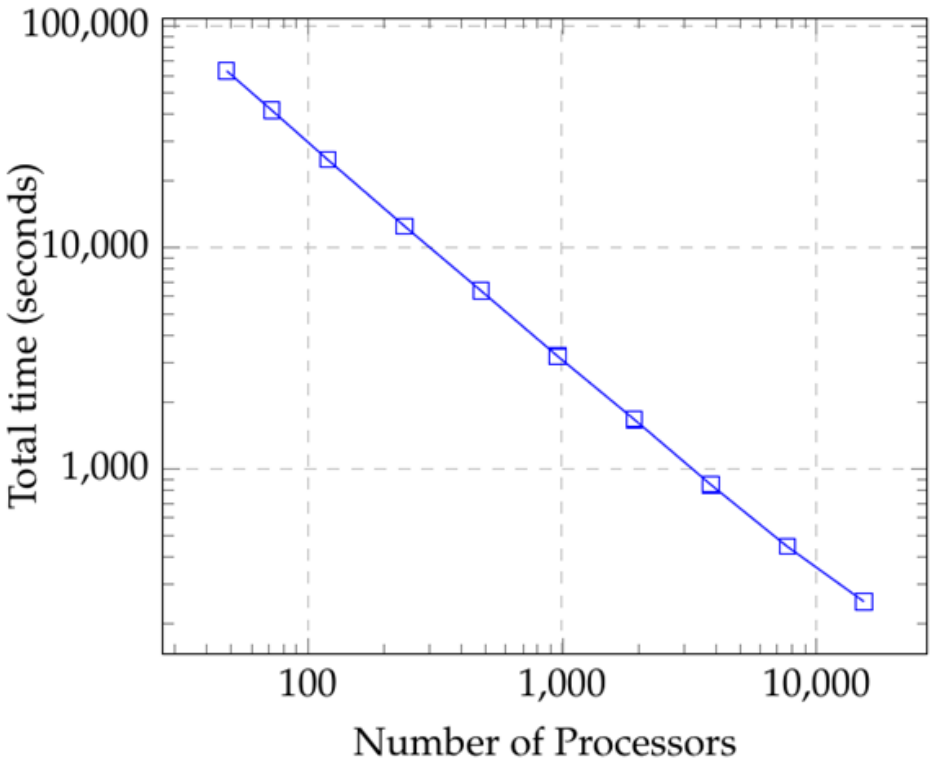
We have used CRAY XC40 system for the computations. We have used 240 to 1536 cores frequently for computations

Parallelization strategies

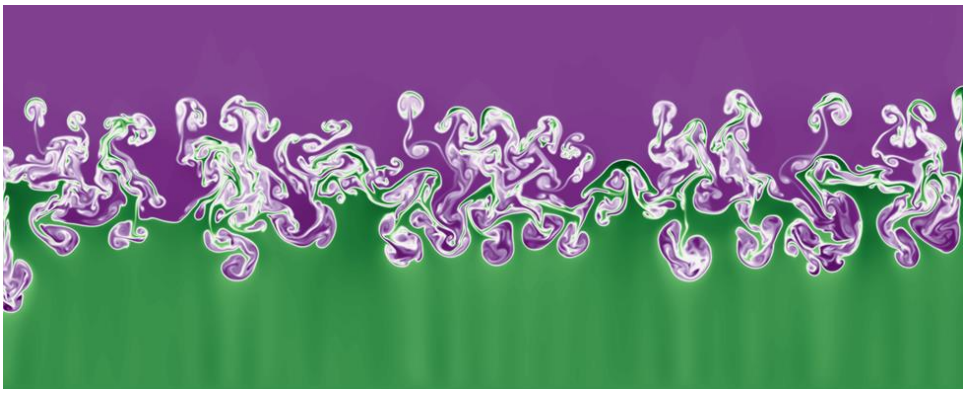
The code uses popular open source code PETSc for parallelization. The code is based on domain decomposition model and uses MPI standard under the hood. Since cray system provides PETSc modules by default, compiling and running the code is quite straightforward.

Performance

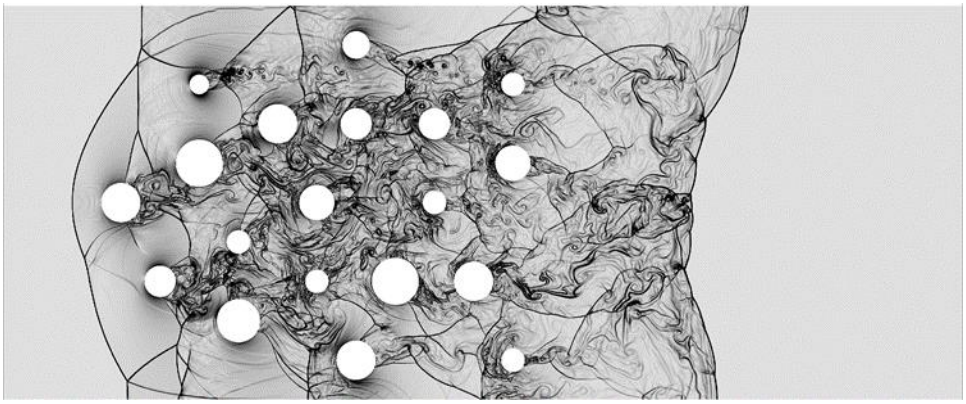
We have performed scalability tests on the code and obtained reasonably good scalability up to 15000 cores.



Demonstration results



Multimode Rayleigh-Taylor Instability. Density contours with violet and green colours indicating the heavier and lighter fluids, respectively with the gravity pointing downwards.



Impact of a Mach 2.4 shock right moving shock in air with a water cylinder. Colours indicate exponentially spaced normalized density gradient contours

Publications

1. Das, A., Shukla, R. K., & Govardhan, R. N. (2022). Contrasting thrust generation mechanics and energetics of flapping foil locomotory states characterized by a unified *St-Re* scaling. *Journal of Fluid Mechanics,* 930, A27.
2. Kumar, A., Rehman, N.M.A., Giri, P., & Shukla, R. K. (2021). An asymptotic theory for the high-Reynolds-number flow past a shear-free circular cylinder. *Journal of Fluid Mechanics,* 920, A44.
3. Ghatage, D., Tomar, G. & Shukla, R. K. (2020). Thermostat-induced spurious interfacial resistance in non-equilibrium molecular dynamics simulations of solid–liquid and solid–solid systems. *The Journal of Chemical Physics*, 1*53*(16), 164110.

K. Ganapathy Ayappa (Chemical Engineering)

Ayappa and co-workers have been using the HPC systems to carry out molecular dynamics simulations to study the interaction of large protein molecules implicated in bacterial infections. These proteins, referred to as pore forming toxins undergo large conformational changes prior to assembly and pore formation on the target membranes. The conformational changes associated with these proteins are complex and we have been studying the free energy of these transitions. We have developed a new coarse grained force-field based on dissipative particle dynamics simulations to study protein secondary structure changes. In other works in collaboration with the Maiti laboratory, we are examining the dynamics of CO_2 molecules in polymer based membranes for carbon capture and sequestration.

SERC's resources: the particular SERC's HPC resource used, the number of cores employed for your problem (2 lines)

All-atom molecular dynamics simulations of membrane-protein systems range for 1 Lakh to 5 Lakh atoms with 240 – 480 cores on the Cray XC 40

Parallelization strategies employed (4 lines)

Simulations are carried out using LAMPPS and GROMACS MD engines. Parallelization for the GROMACS is carried out using GMX_MPI. Our simulations are CPU based.

Performance: Typical execution times in SERC HPC systems and comparisons to the times taken for your runs otherwise (e.g., any other facility, your lab's systems) (2-4 lines)

Typical HPC execution times in the molecular dynamics simulations for systems consisting of about 1 lakh atoms range from 80 – 100 ns/day across 10 compute nodes (240 cores). This is about 2-3 times faster than our in-house computing resources.

CoVid 19 research using HPC simulations: The last two years (2020 and 2021) also saw the spread of CoVid-19 and various research efforts related to the pandemic. It will be great if you can add a section on research related to CoVid-19, if any, using HPC simulations on SERC resources. We can target to have such collated information in venues like IISc Kernel magazine. (6 -10 lines).

We have initiated a study on the interaction of the SARS-Cov2 fusion peptides with mammalian plasma membranes in order to understand the influence of membrane cholesterol on fusion peptide binding.

Publications

1. A Generic Force Field for Simulating Native Protein Structures Using Dissipative Particle Dynamics, Rakesh Vaiwala, K. G. Ayappa, ***Soft Matter***, 17, 9772-9785 (2021). https://doi.org/10.1039/D1SM01194D
2. Pore Forming Protein Induced Biomembrane Reorganization and Dynamics: A Focused Review, Ilanila Ilangumaran Ponmalar, Nirod K. Sarangi, Jaydeep K. Basu and K. Ganapathy Ayappa, ***Frontiers in Molecular BioSciences,*** 8:737561, (2021) https://doi.org/10.3389/fmolb.2021.737561
3. Hydrophobic Gating and 1/f Noise of the Anthrax Toxin Channel, Goli Yamini, Subbarao Kanchi, Nnanya Kalu, Sanaz Momben Abolfath, Stephen H. Leppla, K. Ganapathy Ayappa, Prabal K. Maiti and Ekaterina M Nestorovich, ***Journal of Physical Chemistry B*** 125, 21, 5466–5478 **(**2021). https://doi.org/10.1021/acs.jpcb.0c10490
4. Evaluating Coarse-Grained MARTINI Force-Fields for Capturing the Ripple Phase of Lipid Membranes, Pradyumn Sharma, Rajat Desikan and K. Ganapathy Ayappa, ***Journal of Physical Chemistry B,*** 125, 24, 6587–6599 (2021). https://doi.org/10.1021/acs.jpcb.1c03277
5. Predicting Interfacial Hot-Spot Residues that Stabilize Protein-Protein Interfaces in Oligomeric Membrane-Toxin Pores Through Hydrogen Bonds and Salt Bridges, Rajat Desikan, P.K. Maiti and K.G. Ayappa, ***Journal of Biomolecular Structure and Dynamics,*** 39, 20-34 (2021). https://doi.org/10.1080/07391102.2020.1711806
6. Mechanistic Insights into Pore Formation by an a-pore Forming Toxin: Protein and Lipid Bilayer Interactions of Cytolysin A, Pradeep Sathyanarayana, Sandhya Visveswariah, K. G. Ayappa, ***Accounts of Chemical Research***, 54, 120-131 (2021). https://doi.org/10.1021/acs.accounts.0c00551

Book Chapters:

1. Dendrimer: A Novel Nanomaterial, Debabrata Pramanik, Subbarao Kanchi, K. G. Ayappa and Prabal K. Maiti, *Springer Series in Materials Science, Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile***,** Edited by, Sadasivan Shankar, Richard Muller, Thom Dunning and Guan Hua Chen, 284 (2021).
2. Using Multiscale Molecular Dynamics Simulations to Obtain Insights into Pore Forming Toxin Mechanisms, Rajat Desikan, Amit Behera, Prabal Maiti, K. G. Ayappa, in *Methods in Enzymology,* Issue on Pore Forming Toxins, Elsevier, Edited by Alejandro Hueck, (2021)

Contributions to the national/Industry/societal projects due to the executions, and the resulting impact.

With a grant from the National Supercomputing Mission we are in the process of developing methods to carry out dissipative particle dynamics simulations of proteins and develop free energy computation techniques to study protein conformational changes in membrane inserted environments.

PhD, Masters and UG students graduated in 2020 and 2021, whose work is based on the use of SERC HPC resources.

Phd - 1 MTech - 2

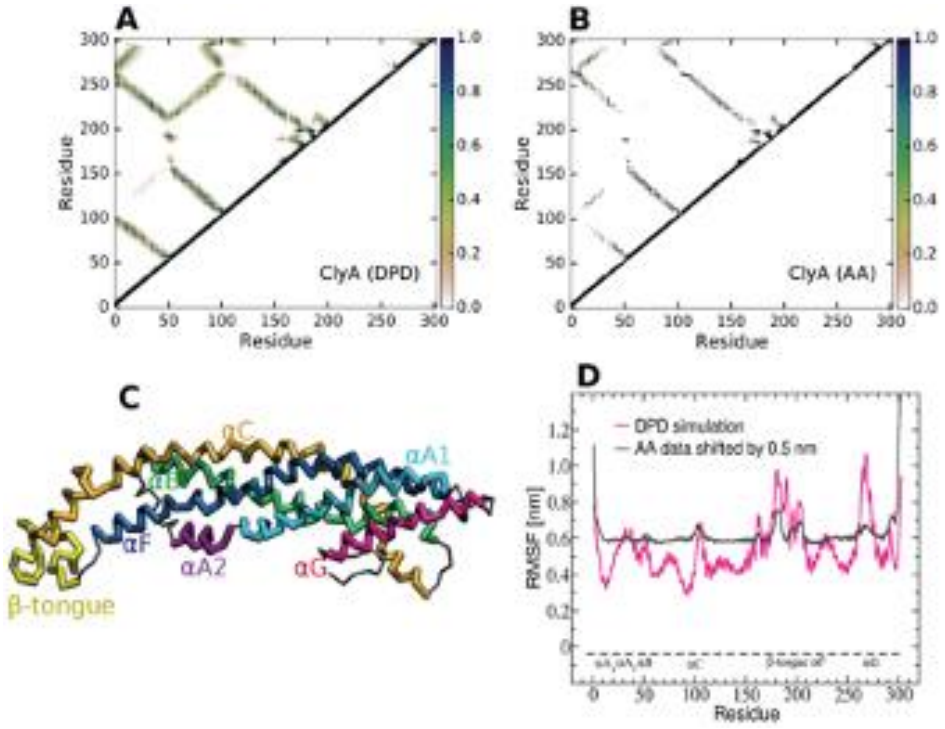


Figure 1: Dissipative particle dynamics (DPD) simulations of the pore forming protein cytolysin A illustrated in C. The contact maps from the DPD simulations (A) are compared with the all-atom simulations (B) and the root mean square fluctuations are compared in D. Data reproduced from Vaiwala and Ayappa, Soft Matter, 17, 9772-9785 (2021). https://doi.org/10.1039/D1SM01194D

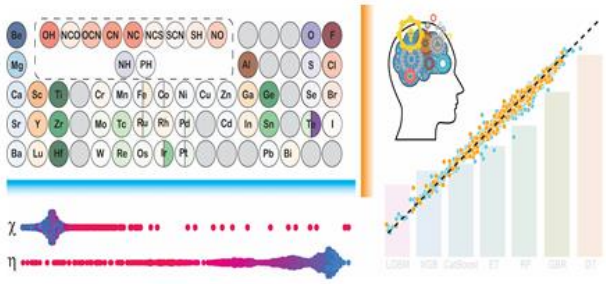
Abhishek Kumar Singh (MRC)

Problem Solved:

Our group is extensively involved in theoretical research in the field of interdisciplinary area of materials science and engineering. Our domain of research includes thermo-electrics, 2D materials, doping, defects, catalysis, optical properties, topological materials, and image processing of structural materials using the first-principles approach and machine learning (ML). Following are the highlights of our research work that uses SERC HPC:

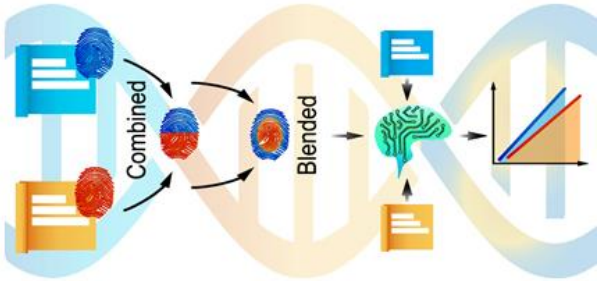
- Machine Learning approach for different material's property prediction from very simple elemental and structural information.

Interpreting 'Black-box' Machine Learning To Guide Materials Discovery



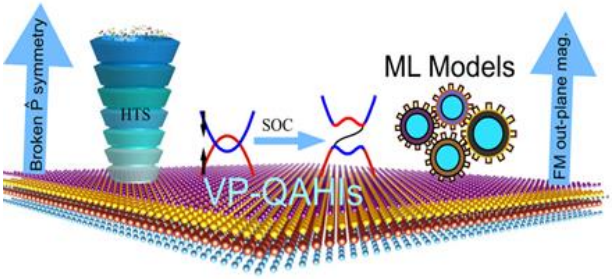
NPJ Comput. Mater. **7**, 197 (2021)

Feature Blending toward ML Models for Property Prediction



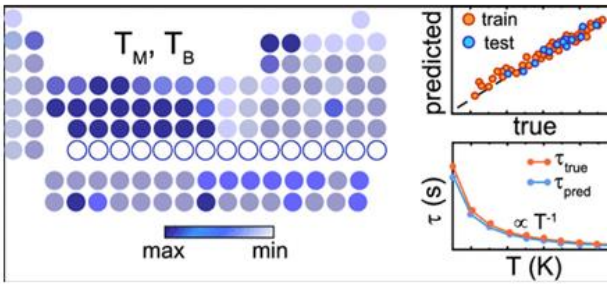
ACS Phys. Chem Au **2**, 16 (2022)

Accelerated Discovery of the Valley-Polarized Quantum Anomalous Hall Effect in MXenes



Chem. Mater. **33**, 6311 (2021)

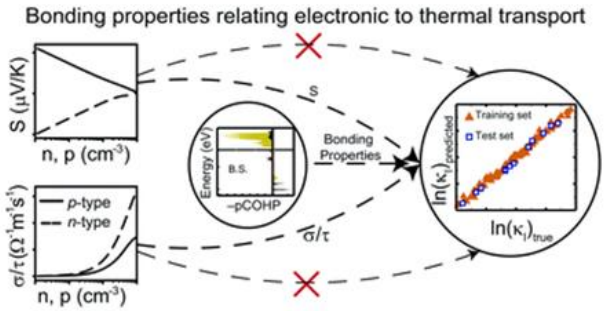
Rapid Prediction of Electron Relaxation Time Using Elemental Representatives



Chem. Mater. **32**, 6507 (2020)

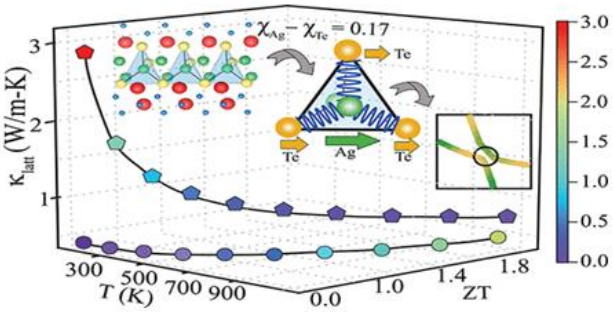
- Engineering of structural symmetry for achieving high thermoelectric performance.

Role of bonding chemistry in connecting electronic and thermal transport by machine learning



Chem. Mater. **32**, 6507, (2020)

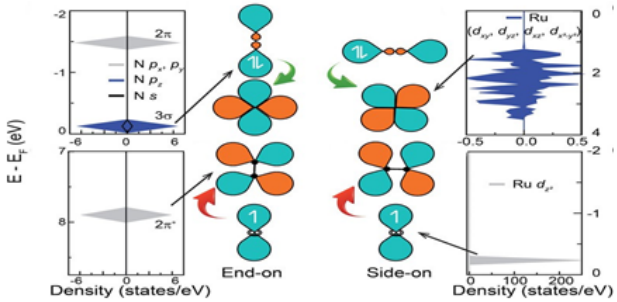
Chemical Bond Hierarchy Leading to Achieve High Thermoelectric Figure of Merit



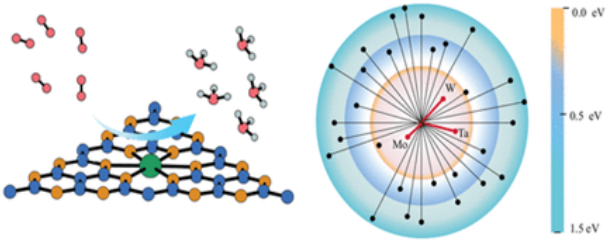
J. Mater. Chem. A **8**, 8716, (2020)

- Intuitive Design Principle of Single-Atom Catalysts for Efficient Electrolytic Nitrogen Reduction.

Rational Design of Single-Atom Catalysts for Enhanced Electrocatalytic Nitrogen Reduction Reaction



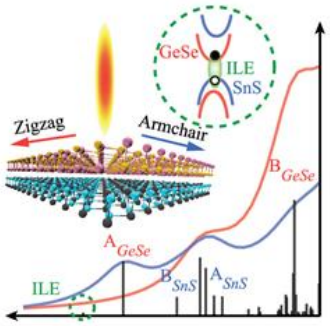
ChemCatChem, **12**, 5456 (2020).



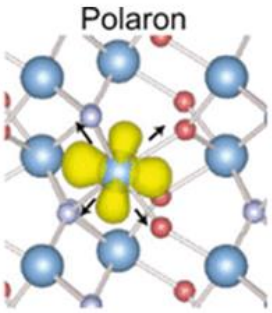
J. Phys. Chem. C **125**, 12585 (2021)

- Engineering of electronic and optical properties of materials via doping, defects and quasiparticle incorporation.

Exciton and Polaron Quasiparticle Dynamics for Oprtical and Electonic Properties

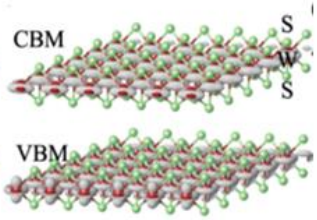


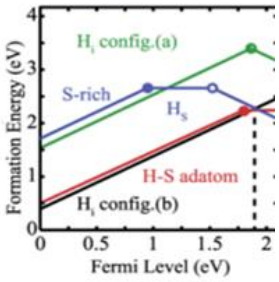
J. Phys. Chem. Lett., 12, 1765 (2021)



J. Phys. Chem. C, 125, 11548 (2021)

Intrinsic Defects and promising dopants in two-dimensional WS_2

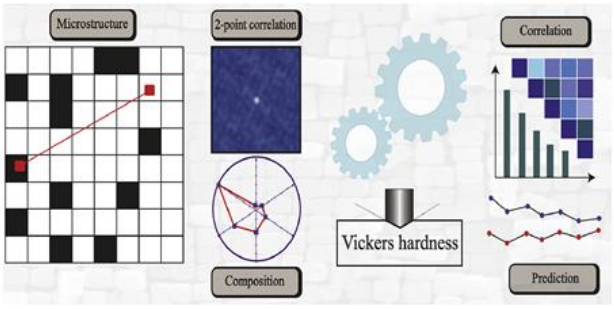




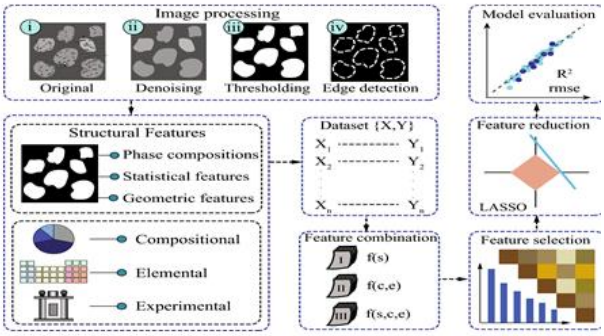
Phys. Rev. Materials, 5, 084001 (2021)

- Establishing structure-property linkages using machine learning and image processing techniques.

Vickers Hardness Prediction Using Advanced Image Processing Techniques And Machine Learning



Acta Mater., 196, 295-303, (2020)



J. Mater. Sci. **55**, 15845 (2020)

Resources:

Our group mainly used the SahasraT (Cray XC40) supercomputer at SERC to carry out Density Functional Theory calculations. We usually used 4 to 10 nodes containing 24 CPU cores each of small and small72 queue. We also ran job using maximum up to 40 compute nodes in medium queue in some cases.

Parallelization:

VASP, Quantum Espresso, WannierTools, ShengBTE parallel codes were used, with both multi-core and multi-node parallelization.

Performance:

The performance speed of the computational facilities at SERC is comparable to our lab cluster. However, we were able to run multiple jobs simultaneously in SahasraT Cray XC40 which would not have been possible using our lab clusters.

CoVid 19 research using HPC simulations: N/A

Outputs:

Publications

1. R. Das, S. Sarkar, R. Kumar, S. D. Ramarao, A. Cherevotan, M. Jasil, C. Vinod, A. K. Singh, and S. Peter, Noble Metal Free Heterojunction Photocatalyst for Selective CO_2 Reduction to Methane upon Induced Strain Relaxation, ACS Catal., 12, 687-697 (2021)
2. R. Kumar, and A. K. Singh, Chemical Hardness-driven Interpretable Machine Learning Approach for Rapid Search of Photocatalysts, npj Comput. Mater., 7, 197 (2021)
3. N. K. Katiyar, S. Dhakar, A. Parui, P. Gakhad, A. K. Singh, K. Biswas, C. S. Tiwary, and S. Sharma, Electrooxidation of Hydrazine Utilizing High-Entropy Alloys: Assisting the Oxygen Evolution Reaction at the Thermodynamic Voltage, ACS Catal., 11, 14000–14007 (2021)
4. S. Satsangi, A. Mishra, and A. K. Singh, Feature Blending: An Approach Towards Generalized Machine Learning Models for Property Prediction, ACS Phys. Chem Au, 2, 16-22 (2022)
5. L. Sharma, N. K. Katiyar, A. Parui, R. Das, R. Kumar, C. S. Tiwary, A. K. Singh, A. Halder, and K. Biswas, Low-cost high entropy alloy (HEA) for high-efficiency oxygen evolution reaction (OER), Nano Res., In press (2021)
6. R. K. Barik, and A. K. Singh, Accelerated discovery of valley polarized quantum anomalous hall effect in MXenes, Chem. Mater., 33, 6311–6317 (2021)
7. A. Singh, and A. K. Singh, Atypical behaviour of intrinsic defects and promising dopants in 2D-WS_2, Phys. Rev. Materials, 5, 084001 (2021)
8. B. Sarkar, A. Parui, A. K. Singh, and K. K. Nanda, Mechanistic study on Nitrogen-doped graphitic carbon-reinforced chromium nitride as durable electrocatalyst for oxygen reduction, J. Mater. Chem. A, 9, 16575-16584 (2021).
9. S. Agarwal, R. Kumar, R. Arya, and A. K. Singh, Rational Design of Single-Atom Catalysts for Enhanced Electrocatalytic Nitrogen Reduction Reaction, J. Phys. Chem. C, 125, 12585–12593 (2021).
10. M. Dey, A. Singh, and A. K. Singh, Formation of Small Electron Polaron in Tantalum Oxynitride: Origin of Low Mobility, J. Phys. Chem. C, 125, 11548-11554 (2021).
11. A. Bhui, M.Dutta, M. Mukherjee, K. S. Rana, A. K. Singh, A. Soni, and K. Biswas, Ultralow Thermal Conductivity in Earth-Abundant $Cu_{1.6}Bi_{4.8}S_8$: Anharmonic Rattling of Interstitial Cu, Chem. Mater., 33, 2993–3001 (2021).
12. N. Maity, P. Srivastava, H. Mishra, R. Shinde, and A. K. Singh, Anisotropic Interlayer Exciton in GeSe/SnS Van der Waals Heterostructure, J. Phys. Chem. Lett., 12, 1765−1771 (2021).

13. Y. Zhou, N. Maity, J. F. Lin, A. K. Singh, and Y. Wang, Nonlinear Optical Absorption of ReS_2 Driven by Stacking Order, ACS Photonics, 8, 405-411, (2021).
14. P. Kumbhakar, M. Mukherjee, A. Pramanik, S. Karmakar, A. K. Singh, C. S. Tiwary, and P. Kumbhakar, Confinement Aided Simultanous Water Cleaning and Energy Harvesting Using Atomically Thin Wurtzite (Wurtzene), Adv. Sustain. Syst., 5, 2000189 (2020).
15. X. Meng, A. Singh, R. Juneja, Y. Zhang, F. Tian, Z. Ren, A. K. Singh, L. Shi, J.F. Lin, and Y. Wang, Pressure Dependent Behavior of Defect-modulated Band Structure in BAs, Adv. Mater., 32, 2001942 (2020).
16. S. Swetlana, N. Khatavkar, and A. K. Singh, Development of Vickers hardness prediction models via microstructural analysis and machine learning, J. Mater. Sci., 55, 15845–15856, (2020).
17. R. Kumar, and A. K. Singh, Electronic Structure Based Intuitive Design Principle of Single-Atom Catalysts for Efficient Electrolytic Nitrogen Reduction, ChemCatChem, 12, 5456-5464, (2020).
18. M. Mukherjee, S. Satsangi, and A. K. Singh, A Statistical Approach for the Rapid Prediction of Electron Relaxation Time Using Elemental Representatives, Chem. Mater., 32, 6507–6514, (2020)
19. N. Khatavkar, S. Swetlana, and A. K. Singh, Accelerated prediction of Vickers hardness of Co- and Ni-based superalloys from microstructure and composition using advanced image processing techniques and machine learning, Acta Mater., 196, 295-303, (2020).
20. T. Pandey, A. Nissimagoudar, A. Mishra, and A. K. Singh, Ultralow Thermal Conductivity and High Thermoelectric Figure of Merit in Mixed Valence In_5X_5Br (X = S, and Se) Compounds, J. Mater. Chem. A, 8, 13812-13819, (2020).
21. P. V. Sarma, T. V. Vineesh R. Kumar, V. Sreepal, R. Prasannachandran, A. K. Singh, and M. M. Shaijumon, Nanostructured Tungsten Oxysulfide as an Efficient Electrocatalyst for Hydrogen Evolution Reaction, ACS Catal., 10, 6753–6762, (2020).
22. K. M. B. Urs, N. K. Katiyar, R. Kumar, K. Biswas, A. K. Singh, C. S. Tiwary, and V. Kamble, Multi-component (Ag–Au–Cu–Pd–Pt) alloy nanoparticle-decorated p-type 2D-molybdenum disulfide (MoS_2) for enhanced hydrogen sensing, Nanoscale, 12, 11830-11841, (2020).
23. Y. Zhou, N. Maity, A. Rai, R. Juneja, X. Meng, A. Roy, Y. Zheng, X. Xu, J. F. Lin, S. K. Banerjee, and A. K. Singh, Y. Wang, Stacking-Order-Driven Optical Properties and Carrier Dynamics in ReS_2, Adv. Mater. 32, 1908311 (2020).
24. R. Juneja, and A. K. Singh, Unraveling the role of bonding chemistry in connecting electronic and thermal transport by machine learning, J. Mater. Chem. A 8, 8716-8721, (2020).
25. N. K. Katiyar, S. Nellaiappan, R. Kumar, K. D. Malviya, K. G. Pradeep, A. K. Singh, S. Sharma, C. S. Tiwary, and K. Biswas, Formic acid and methanol electro-oxidation and counter hydrogen production using nano high entropy catalyst, Mater. Today Energy 16, 100393 (2020).
26. R. Juneja and A. K. Singh, Guided Patchwork Kriging to Develop Highly Transferable Thermal Conductivity Prediction Models, JPhys Materials, 3, 024006 (2020).
27. S. Nellaiappan, N. Katiyar, R. Kumar, A. Parui, K. Malviya, K. Pradeep, A. K. Singh, S. Sharma, C. Tiwary, and K. Biswas, High-Entropy Alloys as Catalysts for the CO_2 and CO Reduction Reactions # Experimental Realization, ACS Catal., 10, 3658-3663, (2020).
28. M. Mukherjee and A. K. Singh, Strong Chemical Bond Hierarchy Leading to Exceptionally High Thermoelectric Figure of Merit in Oxychalcogenide AgBiTeO, ACS Appl. Mater. Interfaces, 12, 8280-8287, (2020).
29. S. Nellaiappan, R. Kumar, C. Shivakumara, S. Irusta, J. A. Hachtel, J. C. Idrobo, A. K. Singh, C. S. Tiwary, and S. Sharma, Electroreduction of carbon dioxide into selective hydrocarbon at low overpotential using isomorphic atomic substitution in copper oxide, ACS Sustainable Chem. Eng., 8, 179-189, (2020)

Students Graduated

Three PhD and two UG students have graduated in the last two years, whose work is based on the use of SERC HPC resources.

Santosh Hemchandra (Aerospace)

Problem

We studied two problems in 2020-21 using explicit filtering large eddy simulations (EFLES) as follows,

1) Reacting flows at gas turbine relevant conditions [1]

Flows in gas turbine combustors are highly turbulent with flow Reynolds numbers (Re) ~ 20,000 – 80,000. The presence of a flame introduces additional physically significant small-scale processes that makes the computation of these types of flows challenging. The explicit filtering approach, developed hitherto for non-reacting flows, is extended to reacting flows. The flame is modelled using a formally reduced chemical kinetic model and adaptive filtering. Scaling chemical source terms to broaden the reaction zone is a key requirement for stable solutions. The new model was applied to a turbulent methane-air lean premixed jet flame. Excellent agreement between LES and the corresponding fully resolved DNS (direct numerical simulation) results have been obtained.

2) Transonic flow past an axi-symmetric hump [3]

These computations were performed as part of the blind CFD validation challenge problem posed by the experimental team of Steve Beresh and co-workers at Sandia national labs, Albuquerque, NM, USA. The challenge was conducted to evaluate the ability of various CFD methods to key predict flow field features like shock position, separation point and re-attachment point, in addition to, time averaged velocity field statistics at several positions for a transonic flow with Mach number 0.875. Our simulations predict the separation and re-attachment locations to within 4% and 7% of the experimental measurements. Additional simulations at M=0.7 clarify the role of the shock in causing separation. We identify partial re-laminarization as a possible explanation for “ring” like structures in the boundary layer near the hump apex in both cases. Further simulations to improve agreement in other aspects (shock position, peak skin friction coefficient) are ongoing.

Resources

We used the SahasraT. Problem 1 used between 6-24 nodes for LES and 350 nodes for the DNS. Problem 2 used between 580-650 nodes for LES

Parallelization

We use MPI parallelization applied to structured multi-block overset meshes.

Performance

Problem 1: LES ~ 24 hrs, DNS ~ 64 hrs.

Problem 2: 72 hrs

Outputs

Publications

1. Datta, A., Mathew, J. and Hemchandra, S., "The explicit filtering method for large eddy simulations of a turbulent premixed flame", *Combustion and flame,* 2022, vol. 237, https://doi.org/10.1016/j.combustflame.2021.111862.
2. Mukherjee, A., Muthichur, N., More, C., Gupta, S. and Hemchandra, S. "The role of the centerbody wake on the precessing vortex core dynamics of a swirl nozzle.", *Journal of engineering for gas turbines and power*, 2021, vol. 143(5) https://doi.org/10.1115/1.4050155
3. Gupta, M., Datta, A., Mathew, J. and Hemchandra, S., "Shock induced transition in a transonic flow past an axi-symmetric hump", 2021, AIAA aviation forum, paper #2021-2756

Typical results

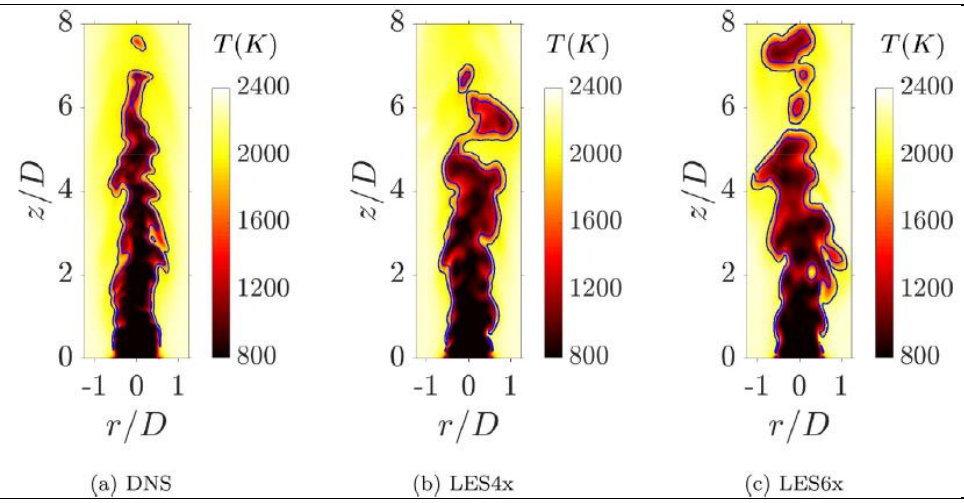


Figure 1: Typical instantaneous temperature field snapshots from DNS and LES simulaitons. CH4-air premixed jet flame with equivalence ratio of 0.8 (Datta et al [1]).

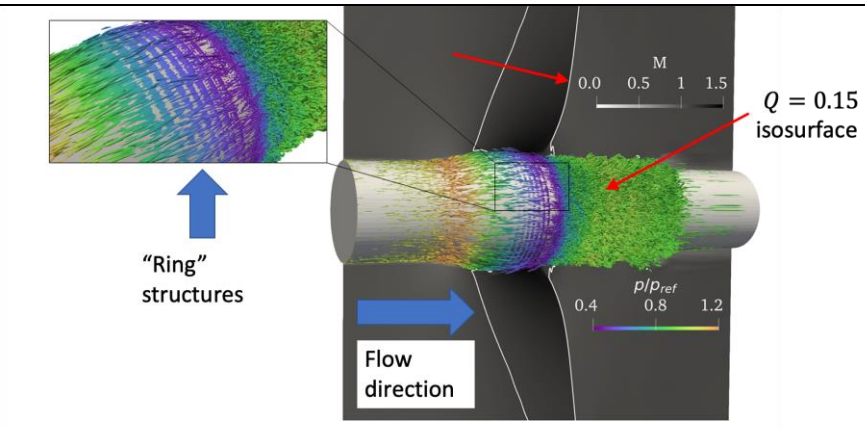


Figure 2: Typical snapshot from flow past an axi-symmetric transonic hump. M = 0.875. The figure shows the supersonic pocket terminated by the shock (red arrow) and "ring" structures (inset), possibly due to partial re-laminarization of the flow (Gupta et al [3]).

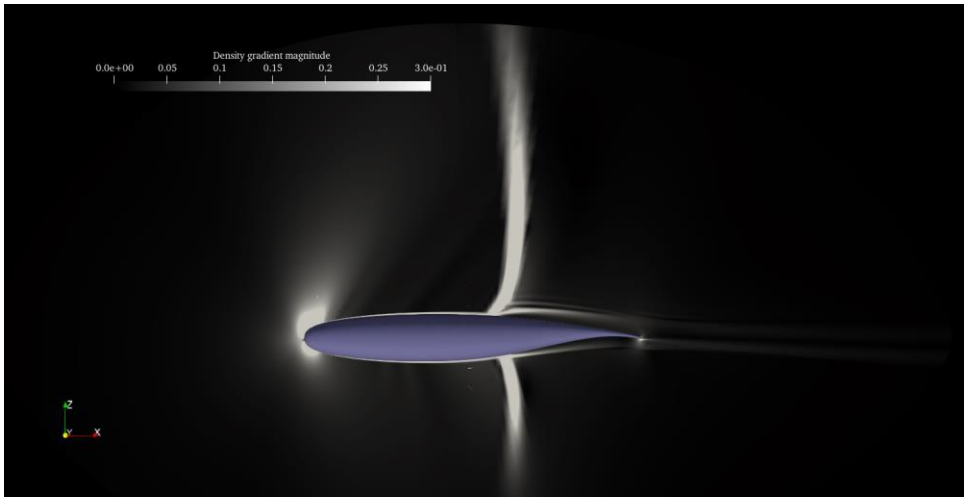
Kartik Venkatraman (Aerospace)

Transonic buffet, buffeting, and flutter in un-swept and swept wing

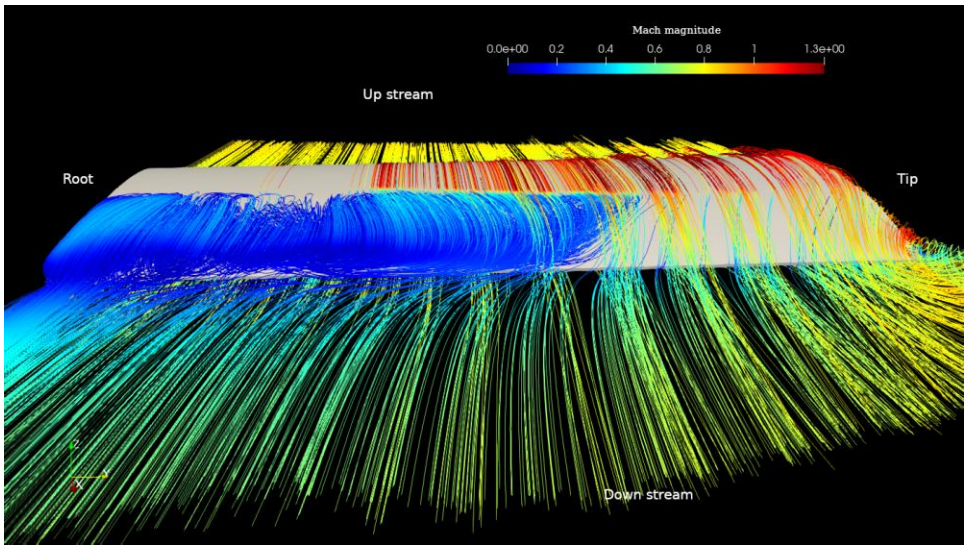
Our group is engaged in numerically predicting transonic buffet, or shock oscillations induced by shock-boundary layer interactions, in finite span wings with supercritical airfoils. Understanding the mechanism that generates these oscillations in finite span wings is critical to reducing unsteady wave drag and increasing fuel efficiency in passenger aircraft.

All simulations were done on SahasraT (Cray XC40) using approximately 500 cores.

The configuration simulated is part of the Aeroelastic Prediction Workshop AePW3 | Home (nasa.gov), High Angle working group.



Numerical schlieren, or density gradient magnitude, of flow captures shock over the surface of the airfoil; M = 0.85, Re_c = 4.48 x 10^6, $\alpha = 5^0$, NASA SC(2)-0414 airfoil, AR = 2.



Flow streamlines over the wing clearly showing the shock induced flow separation and spanwise component of flow; M=0.85, Re_c= 4.48 x 10^6, α=5^0, NASA SC(2)-0414 airfoil, AR=2.

Publications

Magan Singh, Pradeepa Tumkur Karnick, and Kartik Venkatraman, 2022, Transonic buffet and buffeting in the finite span Benchmark Supercritical Wing (BSCW), AIAA Aviation Forum and Exposition, June-July 2022.

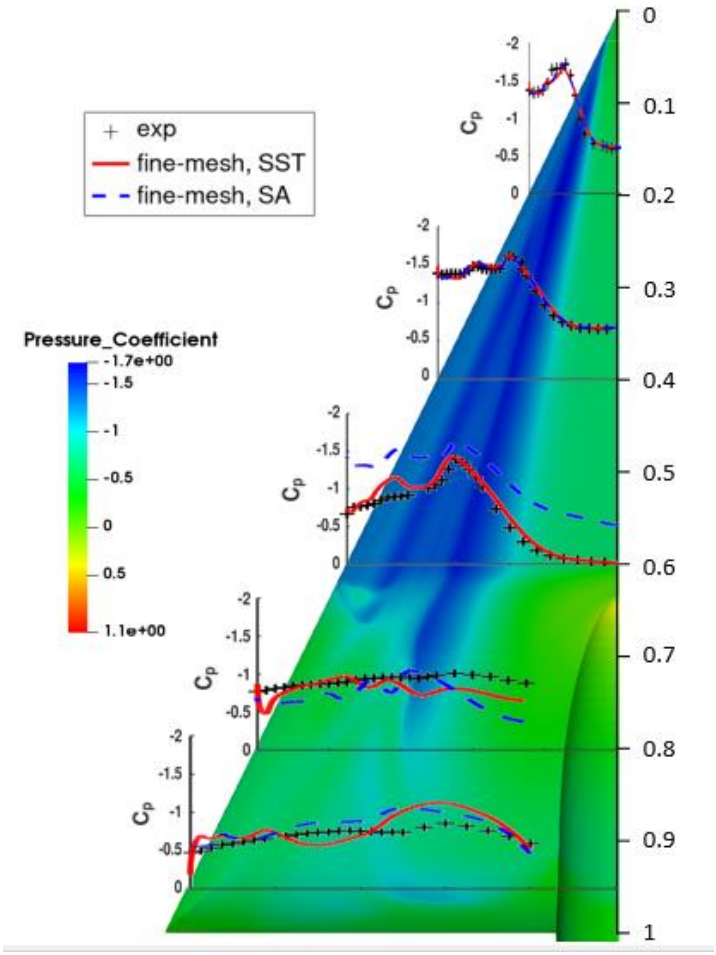
Magan Singh and Kartik Venkatraman, 2022, Transonic buffet in the Benchmark Supercritical Wing: AePW-3 test case, International Forum on Aeroelasticity and Structural Dynamics (IFASD), June 2022.

Shock-vortex-boundary layer interaction of a delta wing in transonic flow

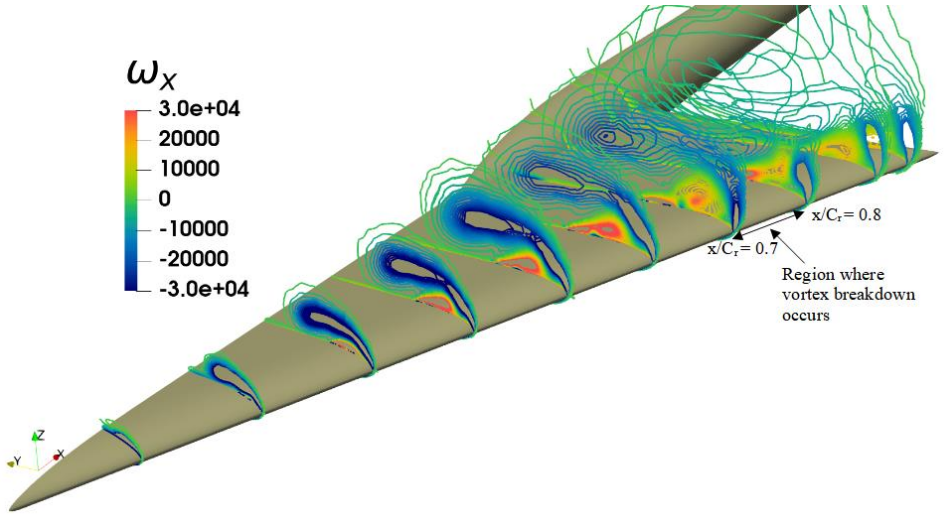
Flow over a delta wing at moderate angles of incidence is vortex dominated with leading edge primary, secondary, and even tertiary vortices. Flow separation and re-attachment is present due to an interplay of geometry of the wing and vortex-boundary layer interaction. Transonic flow brings with it shocks over the surface of the wing that interacts with vorticity and boundary layer leading to shock oscillations and vortex breakdown.

Simulations done on SahasraT (Cray XC40) with approximately 1000 cores.

The configuration simulated was part of the Vortex Flow Experiment (VFE-2) [Institute of Aerodynamics and Flow Technology - Project Background (phase 1) (dlr.de)]



Coefficient of pressure (C_p) contours over the wing and variation at different (x/c_r) stations; M = 0.8, $Re_{\bar{c}} = 6 \times 10^6$, $\alpha = 24.6^0$, Leading edge sweep angle 65^0, Medium radius leading edge flat plat airfoil.



Vorticity contours over the wing at different (x/c_r) stations; M = 0.8, $Re_{\bar{c}}$ = 6 x 10^6, α = 24.6^0, Leading edge sweep angle 65^0, Medium radius leading edge flat plat airfoil.

Publications

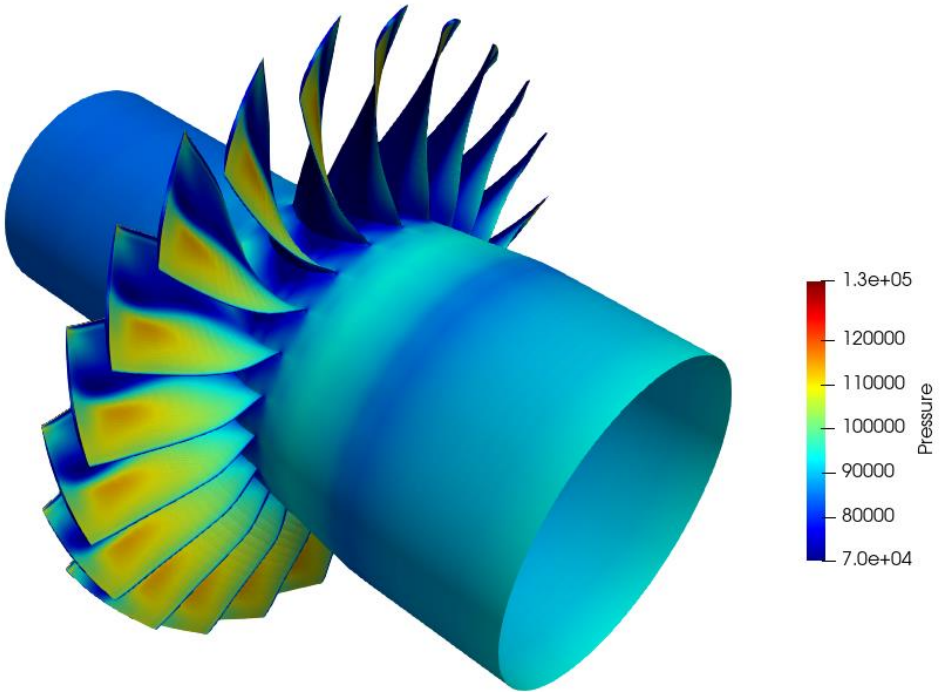
Adithya Mayya, Pradeepa Tumkur Karnick, and Kartik Venkatraman, 2022, Shock vortex interactions and transonic buffet over a flexible delta wing, AIAA Aviation Forum and Exposition, June-July 2022.

Adithya Mayya and Kartik Venkatraman, 2022, Transonic flutter in a delta wing, International Forum on Aeroelasticity and Structural Dynamics (IFASD), June 2022.

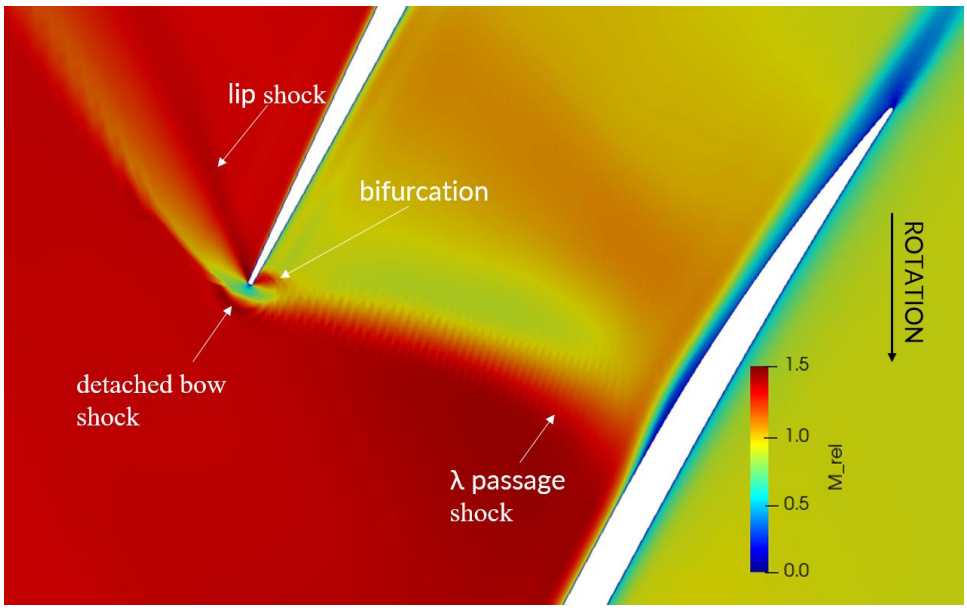
Transonic buffet in an axial flow fan

Axial flow fan in turbofan engines in commercial and military flow aircraft operate in transonic flow conditions. Transonic shock oscillations can lead to a drop in fan efficiency and pressure ratio across the fan. Full annulus URANS simulations of the NASA Rotor 67 axial flow fan are performed at design point (peak efficiency) and off-design (close to stall) conditions.

Simulations done on SahasraT (Cray XC40) with approximately 1000 cores.



Pressure contours over the axial flow fan. The computational domain is also shown. Design rotational speed 16043 rpm; blade tip speed 429 m/s, mass flow rate of 33.25 kg/s; total pressure ratio 1.63.

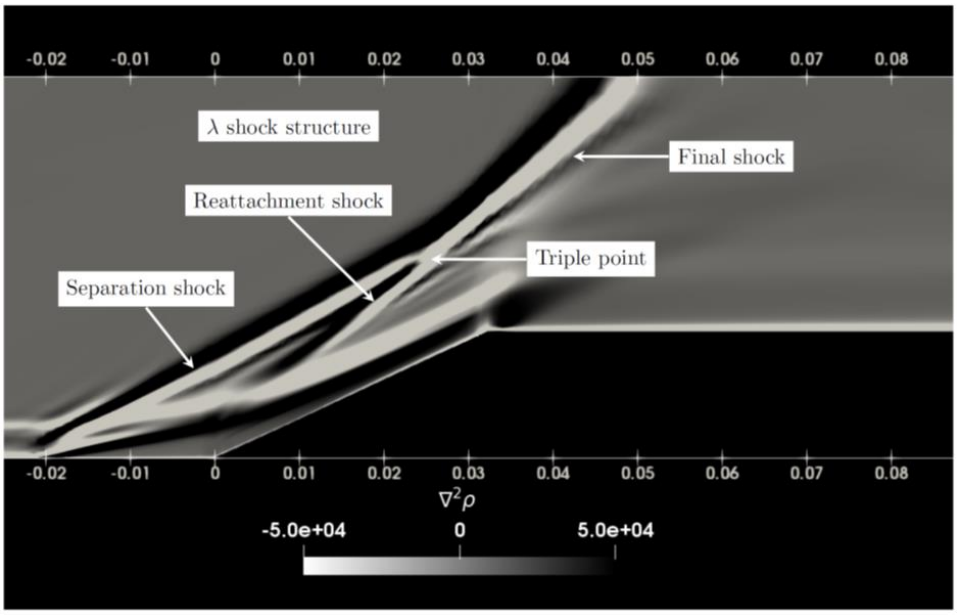


Shock structure at 30% span from fan shroud. Design rotational speed 16043 rpm; blade tip speed 429 m/s, mass flow rate 33.25 kg/s; total pressure ratio 1.63.

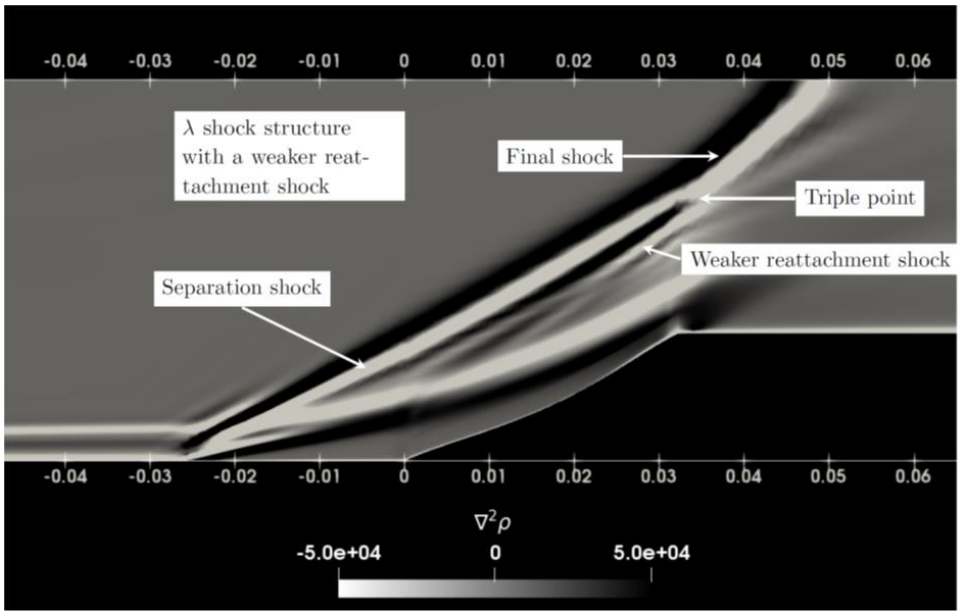
Supersonic flow over a compression-expansion ramp

The compression ramp forms the basis of intakes in hypersonic air breathing flight vehicles. The supersonic free stream flow is de-accelerated and compressed before it enters the scramjet for combustion. Aeroelastic and aerothermoelastic effects can influence the mass flow and compression ratio characteristics by manipulating the shock location and shock structure over the compression ramp.

Simulations done on SahasraT (Cray XC40) with approximately 500 cores.



Shadow graph ($\nabla^2\rho$) showing shock structure over a rigid compression-expansion corner. M = 2.9, Re_δ = 1.48 x 10^5, Ramp angle 25^0.



Shadow graph ($\nabla^2\rho$) showing shock structure over a flexible compression-expansion corner. M = 2.9, Re_δ = 1.48 x 10^5, Ramp angle 25^0, $E/\rho_\infty U_\infty$ = 3.18 x 10^3.

Publication

Sangeet Sourav Sunderroy, Pradeepa Tumkur Karnick, and Kartik Venkatraman, 2022, Shock boundary layer interactions in a supersonic flow over a flexible compression ramp, AIAA Aviation Forum and Exposition, June-July 2022.

Prof. E. D. Jemmis (IPC)

Research:

Our research focuses on understanding the chemistry of molecules and materials at their atomic level using different theoretical techniques. Depending on the problem, we use various methods ranging from semi-empirical extended Hückel method to advanced electronic structure methods. A special emphasis is placed on understanding the evolution of chemistry; from organic to organometallic chemistry; single molecule to a periodic system; polymorphs of elements and their compounds. Apart from getting numbers from the calculations, we focus on why the number turns out to be the way they are and how to engineer the system in a desired direction termed “Orbital Engineering”.

Current emphasis of Research is in the following areas:

a. Chemistry of elemental boron, boron clusters, boranes, metallaboranes and metal borides, 2D-materials such as borophenes and 3D-Borophites.
b. Transition metal organometallics, activation of small molecules, C-H bond activation, alkene hydrosilylation.
c. Aromaticity involving pseudo π* MOs in inorganic systems

d. H-bond, and other weak interactions across the periodic table
e. Chemistry of heavier main group elements
f. Understanding reaction mechanisms using Born-Oppenheimer Molecular Dynamics/ Direct Dynamics.

SERC Resources and Experiments:

Molecular electronic structure calculation (Gaussian 16), solid-state calculations (VASP), and *ab-initio* molecular dynamics calculations (CP2K), are performed using SahasraT. The number of node count varies from 5 to 20. Parallelization strategy is used to enhance the performance of the codes except in Gaussian calculations. Most of the jobs generally take two to three days to complete, as the number of atoms in most of the cases is more than 100. 700 thousand core hours of SahasraT were used. The lab has also used Gaussian 09 program package installed in dell, delta and tyrone clusters.

Performance:

Particularly, Delta cluster with 32 cores and the new Roddam Narasimha Cluster with 48 cores are relatively faster than our home and department cluster with 8 processors (max limit per job).

Output:

In addition to presenting the research work and our method of research in several on-line workshops and conferences the following articles were published. These results of the last two years also were accepted by SERB, DST. The agency extended the Year of Science Chair which helps in paying the computational charges at SERC.

1. Orbital Engineering in Chemistry. E. D. Jemmis, S. Ghorai. *Isr. J. Chem.* 61 (2021) 1-14.
2. Metal stabilized [B8H8]2- derivatives with dodecahedral structure in solid- and solution-state: [(Cp2MBH3)2B8H6], (Cp = η5-C5H5; M = Zr (1-Zr) and Hf (1-Hf)). S. Kar, S. Bairagi, G. Joshi, E. D. Jemmis, S. Ghosh. *Chem. A Eur. J.* 27 (2021) 15634-15637.
3. Comparison of RNC coupling and CO coupling mediated by Cr-Cr quintuple bond and B-B multiple bonds: Main-group metallomimetics. S. Ghorai, R. Meena, A. Joseph, E. D. Jemmis. *J. Phys. Chem. A* 125 (2021) 7207-7216.
4. Reversing Lewis Acidity from Bismuth to Antimony. D. Sharma, S. Balasubramaniam, S. Kumar, E. D. Jemmis, A. Venugopal. *Chem. Commun.* 57 (2021) 8889-8892.
5. Borophenes: Insights and Predictions From Computational Analyses. N. Karmodak, E. D. Jemmis, B. I. Yakobson. *2D Boron: Boraphene, Borophene, Boronene, Springer International Publishing* (2021) 27-49.
6. A Neutral Three-Membered 2π Aromatic Disilaborirane and its Unique Conversion to a Four-Membered BSi2N-Ring. S. K. Sarkar, R. Chaliha, M. M. Siddiqui, S. Banerjee, A. Münch. Herbst-Irmer, D. Stalke, E. D. Jemmis, H. W. Roesky. *Angew. Chemie - Int. Ed.* 59 (2020) 23015-23019.

7. Electrophilic Organobismuth Dication Catalyzes Carbonyl Hydrosilylation. R. Kannan, S. Balasubramaniam, S. Kumar, R. Chambenahalli, E.D. Jemmis, A. Venugopal. *Chem. - A Eur. J.* 26 (2020) 12717-12721.
8. DFT Study of C-C and C-N coupling on a quintuple-bonded Cr2 template: MECP (Minimum Energy Crossing Point) Barriers Control Product Distribution. S. Ghorai, E.D. Jemmis. *Organometallics.* 39 (2020) 1700-1709.
9. Trans-Influence in Heavy Main Group Compounds: A Case Study on Tris(pyrazolyl)borate Bismuth Complexes. S. Balasubramaniam, S. Kumar, A.P. Andrews, E.D. Jemmis, A. Venugopal. *Eur. J. Inorg. Chem.* 2020 (2020) 2530-2536.
10. Structure and bonding in [L]M(μ-CCR)2M[L] and [L]M(μ-RC4R)M[L]: Requirements for C-C coupling. S. Ghorai, E.D. Jemmis. *Dalton Trans.* 49 (2020) 5157-5166.
11. Continuum in H-bond and Other Weak Interactions (X-Z··Y): Shift in X-Z Stretch from Blue Through Zero to Red. G. Karir, E.D. Jemmis. *J. Indian Inst. Sci.* 100 (2020) 127-133.

Cover Page:

In the year 2020-21, one publication (4) from our lab is featured as the cover page in distinguished journal.

Manpower trained:

Dr. Sagar Ghorai, an Int-PhD student, got doctoral degree during this period. Minhajul Islam, an IISc-UG student, submitted MS thesis. Another IISc-UG student, Dhruv Lal submitted BS thesis. Simanthini Paul, an IISER Pune Int-MS student, is about to submit MS thesis. Facilities at SERC helped enormously in their work. One int-PhD student and two regular PhD students are continuing their research using SERC facilities. Three postdoctoral fellows are also using the facility for research. Though to a much less degree, several short-term summer research participants get a flavour of computational chemistry research using the facilities at IPC and on occasions from the SERC facilities.

Konduri Aditya (CDS)

Research:

Our research comprises of two aspects: (1) developing scalable numerical methods for partial differential equations solvers for extreme scale, and (2) massively parallel reacting flow simulations to capture key physics relevant to combustion processes in gas turbine and scramjet engines. Below are the details of these projects.

Asynchronous computing for PDE solvers:

Recent advances in computing technology have made numerical simulations an indispensable research tool in understanding fluid flow phenomena in complex conditions at a great detail. Due to the nonlinear nature of the governing Navier-Stokes equations, simulations of high Reynolds number turbulent flows are computationally very expensive and demand extreme levels of parallelism. The current state-of-the-art turbulent flow simulations are routinely being performed on hundreds of thousands of processing elements. At this extreme scale, communication and synchronization between PEs significantly affect the scalability of solvers. Indeed, communication and data synchronization pose a bottleneck in scalability as simulations advance towards exascale computing. In this project, we have developed a novel approach based on widely used finite-difference schemes in which computations are carried out in an asynchronous fashion, i.e., synchronization of data among processing elements is not enforced and computations proceed regardless of the status of communication. This drastically reduces the CPU idle time and results in much larger computation rates and scalability. We show that while standard schemes can remain stable and consistent, their accuracy is significantly reduced. New asynchrony-tolerant schemes coupled with high-order temporal schemes, which can maintain accuracy under relaxed synchronization conditions, have been derived. The efficacy of these schemes has been demonstrated using SahasraT supercomputer (SERC, IISc). We are also working on the extension of this approach to the discontinuous Galerkin (DG) method

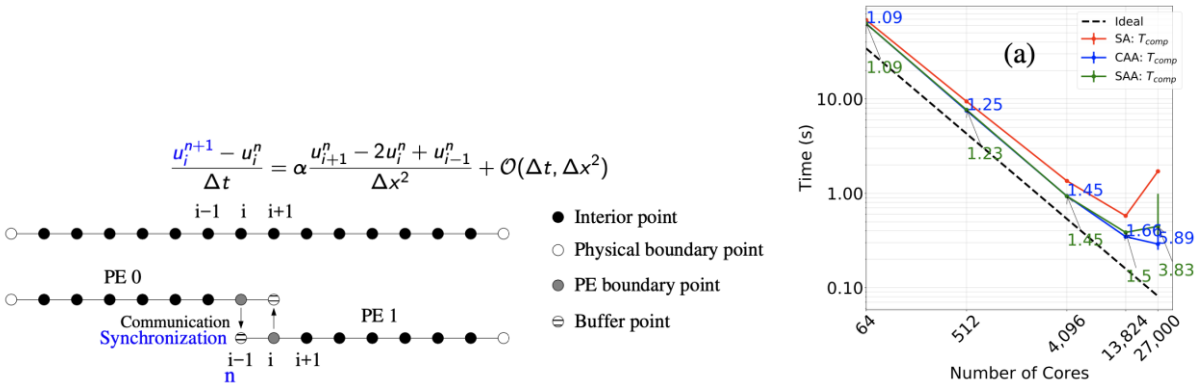


Figure: (left) Schematic illustrating communication pattern in PDE solvers. (right) Strong scaling graph: red line – synchronous implementation, blue and green lines – asynchronous implementations.

Reheat burner for clean energy: A recent study on the operation of a reheat burner (RB) in Ansaldo's GT36 engine with H2-enriched natural gas found that for a H2 fraction >70%, the engine must be derated to achieve the desired combustion characteristics. This was due to a greater contribution of the flame propagation as opposed to the design intended autoignition. In this study, direct numerical simulations are performed in a simplified RB to investigate the effect of blending ratio in CH4-H2-air premixed flames. Three fuel blends comprised of CH4 and H2 at a ratio 0.5:0.5, 0.3:0.7 and 0:1 by volume is considered. At 5 bar the thermo-chemical conditions are chosen to achieve a constant ignition delay time. The results show flame stabilization by autoignition in the bulk flow and by flame propagation in the shear layers immediately downstream of the sudden area expansion. The flame rapidly oscillates in the combustion chamber for pure H2, which is suppressed with addition of CH4. With an increase in CH4 fraction, the flame broadens with a more volumetrically distributed heat release rate.

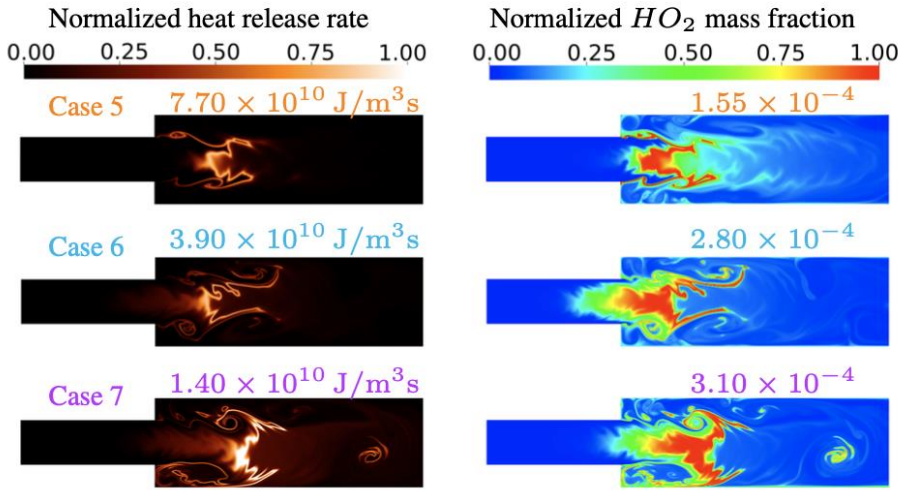


Figure: Instantaneous isocontours of heat release rate and mass fraction of HO2 from three simulations (with 100%, 70% and 50% hydrogen mole fraction, respectively) showcasing the effect of fuel-blending on flame structure.

SERC resources used:

SahasraT supercomputer was extensively used to perform benchmarks for methods development project and to perform production simulation for combustion application. Simulations were performed on core counts ranging from 2000 to 27000.

Parallelization methods:

The code was parallelised based on domain-decomposition technique and communications were facilitated using MPI library. For GPUs, separate functions were developed using CUDA.

Performance:

Our codes have been shown to scale well on the entire machine (upto 30,000 cores).

Outputs:

Rodhiya, A., Gruber, A., Bothien, M. R., Chen, J. H. Aditya, K. (under review). Spontaneous ignition and flame propagation in hydrogen/methane reheat flames: effect of pressure and hydrogen fraction. Proceedings of the Combustion Institute.

Rodhiya, A., Aditya, K., Gruber, A., Chen, J. H. (2021). Simulations of flame structure in a reheat burner: pressure scaling. In AIAA Propulsion and Energy 2021 Forum (p. 3448).

Rodhiya, A., Gruber, A., Chen, J., Aditya, K. (2021). Effect of fuel-blend ratio in methane- hydrogen reheat flames. Bulletin of the American Physical Society, 66.

Rodhiya, A., Aditya, K., Gruber, A., Chen, J. (2020). Pressure scaling of a reheat flame structure. In APS Division of Fluid Dynamics Meeting Abstracts (pp. P03-004).

N. Balakrishnan

Computational Aerodynamics (CAd) Lab

Department of Aerospace Engineering

Simulations carried out on SAHASRAT during 2020 and 2021:

1. Unsteady powered aircraft simulations for a nose mounted propeller aircarft configuration
2. High lift flow simulations
3. DES simulation of supersonic plug nozzle base flows
4. Flow control using synthetic jets

Computational resource used:

Typically, each of the above computations need over 50 million volumes for URANS simulations and about 200 million volumes for the DES simulations. About 8000 cores of CRAY XC 40 platform were engaged for a period ranging from a day to few days for accomplishing the computations listed above. The resource available in the CAd Lab would have required several weeks to complete these runs.

Output:

1. Apurva Anand, *Aerodynamics of Nose Mounted Propeller Aircraft,* M.Tech (Res.) Thesis, July 2020.
2. Publications are under preparation.

Centre for Brain Research (CBR)

Prof. Bratati Kahali's Lab

Research:

There are a total of 48 human samples with a minimum of 30X coverage were analyzed using the whole genome sequencing (WGS) data analysis pipeline. GATK, Sambamba, BWA and samtools are the primary software for performing diverse modules throughout WGS pipeline, including pre-processing of chromosomes by coordinates, mapping to the reference genome and calling individual variants.

Also, processed 366 human whole genome sequencing data to identify population-level genomic variations (called joint-genotyping). Joint genotyping step is achieved with the help of database that efficiently process variants in a single-process multi-data (SPMD) fashion which improving performance while fetching genomic data from tens of thousands of human samples.

Resources:

The 1200 cores of the Sahasrat Cray XC40 were used to parallelize 48 human whole genome sequencing data analysis pipeline, and 24 chromosomes were processed for joint genotyping. The job was submitted in a small high-priority queue of 50 nodes; each node is used with 24 cores.

Parallelization:

Python's Message Passing Interface (MPI) based parallel code helps to process 48 samples and 24 chromosomes in parallel with 50 compute nodes. At each stage of the WGS data analysis pipeline have used the mpi4py python library to run N samples / chromosomes in parallel on N nodes.

Performance:

SahasraT provides "N" nodes to help process "N" human whole genome sequencing data in parallel.

Outputs:

a. Publications: Panda, Abhishek, Krithika Subramanian, and Bratati Kahali. "Implementation of human whole genome sequencing data analysis: A containerized framework for sustained and enhanced throughput." Informatics in Medicine Unlocked 25 (2021): 100684.
b. This work pertains to a contribution to the national GenomeIndia project, funded by the Government of India, DBT.
c. Ongoing PhD student Krithika Subramanian

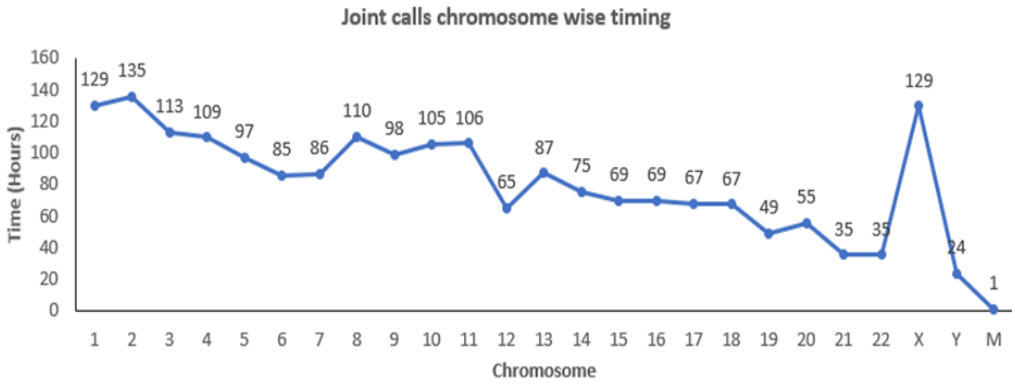


Figure 1: Shows the execution time of population-level genomic variants (Joint-genotyping)

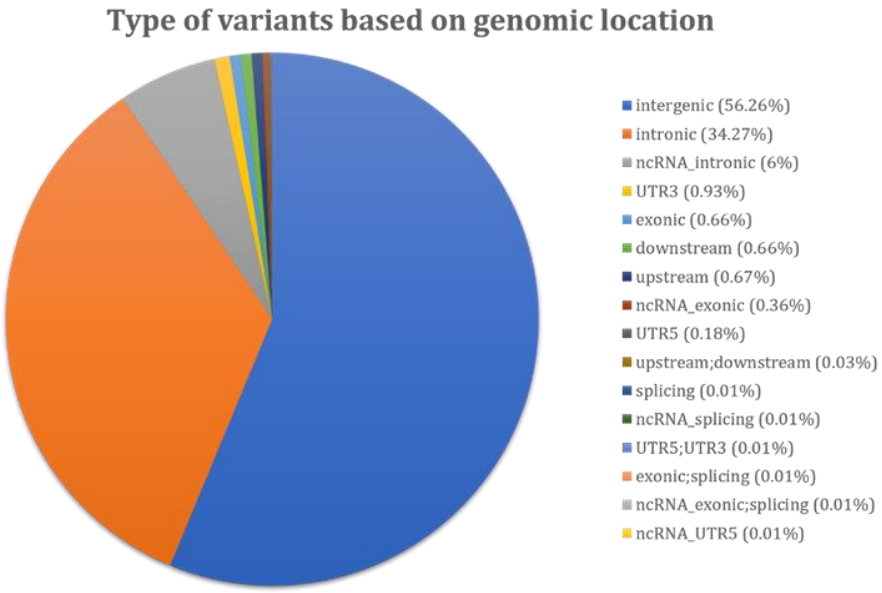


Figure 2: This figure shows the annotation results of 366 human whole genome sequencing data