National PARAM Supercomputing Facility

ANNUAL REPORT

2021

प्रगत संगणन विकास केंद्र

CENTRE FOR DEVELOPMENT OF ADVANCED COMPUTING

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Cover Note

Dear Reader,

Taking forward tradition, National PARAM Supercomputing Facility(NPSF) is proud to present Annual Report for the year 2021. The information in the report is providing both qualitative and quantitative indices of work carried out using NPSF, with an intention to perceive and analyze, both the performance, and in general HPC-AI percolation in India. For the quantitative part, system utilization metrics recorded over the year are incorporated, presenting assorted views of varying utilization aspects. For qualitative part, more specially the scientific outcome of utilization, we have participation from HPC/AI user community wherein information regarding PhDs, Publications and Work Reports are included verbatim.

We would highly appreciate your say on report attached and NPSF in toto, for which you may write to `npsf-outreach@cdac.in` email address.

Happy Computing!

Regards
NPSF

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आवरण पत्र

प्रिय पाठक गण,

अपनी परंपरा को आगे बढ़ाते हुए, एनपीएसएफ वर्ष 2021 की वार्षिक रिपोर्ट प्रस्तुत करते हुए गौरवान्वित महसूस कर रहा हैं। रिपोर्ट में दी गई जानकारी गुणात्मक और परिमाणात्मक दोनों प्रकार के कार्यों की जानकारी प्रदान करती है, जिसे समझने और विश्लेषण करने के साथ ही भारत में आम एचपीसी/एआई परिशोधन करने संबंधी, इन दोनों प्रदर्शनों के उद्देश्य से परम सुपरकंप्यूटिंग सुविधाओं के उपयोग से संपादित किया गया है। परिमाणात्मक भाग के रूप में, वर्ष के दौरान की गई प्रणाली उपयोगिता कार्यों को शामिल किया गया है, और इसके माध्यम से अलग-अलग उपयोगिता पहलुओं के समावेशी दृष्टिकोणों को शामिल किया गया है। गुणात्मक भाग की बात करें, तो विशेष रूप से उपयोगिता के वैज्ञानिक परिणामों को शामिल किया गया है, जहां हमने एचपीसी / एआई समुदाय की ओर से भागीदारी की है। साथ ही इसमें हमारे द्वारा पीएचडी, प्रकाशन और कार्य रिपोर्टों के बारे में जानकारी दी गई है।

इस रिपोर्ट पर आपकी अमूल्य प्रतिक्रिया, सुझावों आदि से हमें अति प्रसन्नता होगी। आप अपने सुझाव, विचार आदि सहर्ष हमें npsf-outreach@cdac.in पर ईमेल कर सकते हैं।

शुभ कंप्यूटिंग, सशक्त कंप्यूटिंग!

भवदीय,

एन.पी.एस.एफ.

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Col. A. K. Nath (Retd.)
Director General, C-DAC, Pune

Message from Director General

I am proud to place this exclusive report on usage statistics and activities carried out on National PARAM Supercomputing Systems for the year 2021.

The scale and complexity of modern technologies and scientific areas make High Performance computing (HPC) increasingly important. Supercomputers are about to enter a new era. What will be more exciting is the convergence of AI and HPC. Industry stalwarts are working towards ecosystems to create a common HPC Infrastructure optimized to run diverse HPC, Big-Data, and AI workloads. This can improve, resource utilization and cost efficiency in a better way.

This year National Supercomputing infrastructure gained substantial momentum with the addition of three 838TF HPC facilities namely PARAM Utkarsh at C-DAC Bangalore, PARAM Seva at IIT Hyderabad, and PARAM Smriti at NABI Mohali. The recently installed PARAM Pravega (3.3PF) at IISc Bengaluru will be released for user access soon. Further to this, large supercomputing systems with a computational power of 1.66 PF at IIT Roorkee will be commissioned soon. PARAM Seva at IIT Hyderabad was inaugurated by Hon. Union Minister Shri Dharmendra Pradhan and PARAM Smriti at NABI Mohali was inaugurated by Hon. Union Minister of State Dr. Jeetendra Singh, during this year.

It is heartening to see that the facilities, PARAM Siddhi (210 AI PF), PARAM Yuva-II (529TF), PARAM Bio-Embryo(100TF), and PARAM Bio-Inferno (150TF) at C-DAC Pune, PARAM Shivay (838TF) at IIT(BHU) Varanasi, PARAM Brahma (1.7 PF) at IISER Pune, PARAM Shakti (1.66PF) at IIT Kharagpur, PARAM Yukti (1.83 PF) at JNCSAR Bangalore, PARAM Sanganak (1.66 PF) at IIT Kanpur are being very well utilized. More than 3 million computational jobs were executed on the PARAM Systems across the country till December 2021. The systems have been used by more than 2200 users from nearly 100 academic and scientific institutions.

The National Supercomputing systems are catering to the scientific community in an extensive manner by making state-of-the-art compute infrastructure and software ecosystems available to researchers and scientists. Many application areas such as flood prediction, seismic-based oil exploration, urban air modelling, CFD simulations, life sciences, and AI/ML/DL have benefitted from the PARAM Supercomputing Systems.

Most importantly, collaboration with premier scientific & engineering organizations will certainly help the HPC team at C-DAC in overcoming the challenges related to the next generation of Exascale systems development.

I would like to thank the HPC teams for their efforts in the deployment and operational support of all PARAM systems 24/7, even during COVID-19 pandemic challenges.

I wish you all the success in your future endeavors!

Col. A. K. Nath (Retd.)
Director General, C-DAC

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Vinodh Kumar M.
Senior Director & HoD,
HPC-I&E Group, C-DAC, Pune

Message from Head of Department

Year 2021 was marked significant changes for the National PARAM Supercomputing Facility(NPSF). I am delighted to present the Annual Report -2021 with highlights of the newly commissioned PARAM Siddhi-AI supercomputer. NPSF feels proud to present the combined efforts to manage the data-centers of PARAM Yuva-II and PARAM Siddhi-AI, which have served various academia and researchers to solve their complex HPC-AI problems. Several benchmark HPC and AI applications have shown successful execution and deployment on NPSF resources. On the one hand, where the HPC users community has shown their immense interest in leveraging the GPU technology of PARAM Siddhi-AI, the other hand, AI applications benefit from the parallel computation training of complex neural networks in a shorter time. NPSF adopted a balanced approach in provisioning HPC resources to both users.

Since PARAM Siddhi-AI commissioning, the NPSF team takes pride in their achievement in providing support to over 1448 users from 158 institutions. The total number of projects being executed is 391, with 100% system availability of PARAM Yuva-II , whereas the PARAM Siddhi-AI system availability was 96.93%, with planned downtime 0.05% and unplanned downtime 3.02%.

I believe this Annual Report 2021 will give a new insight to the HPC-AI users with the presentation of NPSF systems at the various potential matrix.

Vinodh Kumar M.
Senior Director & HoD (HPC-I&E Group)
C-DAC, Pune

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About NPSF

1.1 Introduction

The National PARAM Supercomputing Facility (NPSF) is a result of more than two and half decade effort of Research and Development (R&D) in High Performance Computing (HPC) since C-DAC's inception. The National PARAM Supercomputing Facility was setup in 1998 at C-DAC, Pune with a mandate to offer state-of-the-art High Performance Computing systems and resources to the scientific user community of various academic and research institutes, help them with the know-how and usage of such systems and proliferate HPC awareness in the country.

The supercomputing initiatives PARAM 10000, PARAM Yuva, PARAM Yuva II and now PARAM Siddi-AI at National PARAM Supercomputing will continue to empower our scientists and researchers with state-of-the-art supercomputing facilities and enable them to carry out cutting-edge research in their respective domains.

PARAM Siddhi-AI

PARAM Siddhi-AI is a high performance computing-artificial intelligence (HPC-AI) computing resource and by far the fastest supercomputer developed in India with Rpeak of 6.5 PFlops (DP) and 4.6 PFlops Rmax (Sustained). PARAM Siddhi-AI system ranked 62nd in the Top500 list

of supercomputers in the world published in November 2020 during Supercomputing Conference 2020 (SC 20) at United States.The system is based on the NVIDIA DGX SuperPOD™reference architecture.The system was released in production mode on 23rd August, 2021 .

PARAM Yuva II

In order to keep abreast with the recent trends in HPC with the accelerator/co-processor technology, an upgrade of PARAM Yuva was planned. This upgraded system called PARAM Yuva II, launched in February 2013, was among the latest addition to the series of prestigious PARAM series of supercomputers built in India. PARAM Yuva II was among the first HPC systems in the country using Intel Xeon Phi along with Intel Xeon for achieving its computing power. With this launch, C-DAC also becomes the first R&D institution in India to cross the 500 TF milestone.

PARAM Yuva

The PARAM Yuva (henceforth referred as PARAM Yuva I), which was built and launched in 2008. It was 54 TF system and was ranked 69th in the Top500 list of Supercomputers released in November 2008 at the Supercomputing Conference in Austin, Texas, United States.

PARAM 10000

PARAM 10000 was launched in 1998 with 100 GFlops peak performance and set the path for future developments to come.

A typical system would contain 160 CPUs and be capable of 100 GFLOPS but, it was easily scalable to the TFLOP range, which was exported to Russia and Singapore.

Technical Affiliation Scheme of NPSF

The users from various Universities, IITs and other R&D institutions have the advantage of the reliability and availability associated with National Knowledge Network(NKN) for accessing

computing resources at NPSF. The scientific community use this computing facility through the Technical Affiliate Scheme of NPSF, C-DAC. Under this, the Chief Investigator (Faculty/Scientist at University/Institute/R&D Lab) enrolls as Technical Affiliate, the researcher along with his/her student(s)/collaborator(s) can get user accounts on NPSF resources and avail computing time for their research work. Prospective users can send their queries to *npsfhelp@cdac.in*.

1.2 PARAM Systems

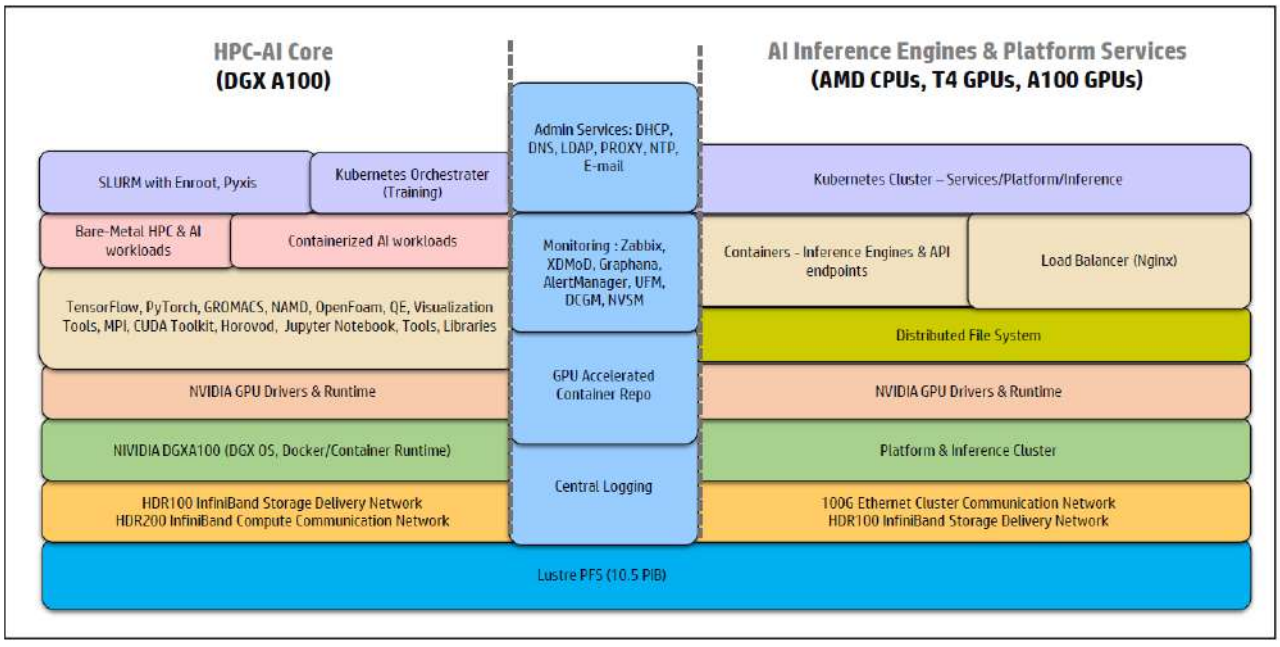
1.2.1 PARAM Siddhi-AI

System Specification	Peak Perf. 210 Petaflop (AI) Rpeak of 6.5 PFlops and 4.6 PFlop Rmax (Sustained Dual Precision) 42 nos. of NVIDIA DGX-A100 nodes Inferencing nodes with NVIDIA Tesla T4 GPUs 8x NVIDIA A100 Tensor Core GPUs each node 320 GB GPU memory/node Infiniband HDR Director Switch (Mellanox CS 8500) Multirail : 8 x 200 gbps (HDR) for compute and 2 x 100 gbps (HDR 100) for storage 10.5 PiB storage with 250 GB/s throughput 500 TiB Flash-based storage and 10 PiB Disk-based storage
AI-HPC Software & NGC	Nvidia NGC (Nvidia GPU Cloud) Software Containers AI frameworks containers - TensorFlow, PyTorch, Keras, TensorRT, MNTK,Theano,XGBoost etc. Deep Learning SDK Container -DeepStream, TensorRT Big-Data and ML, cuGraph Containers – RAPIDS HPC Software Containers - GROMACS, NAMD, GAMESS, LAMMPS, VMD, CHROMA, MATLAB Visualization Container - Paraview CUDA Container Setup of Kubernetes & container platform with NVidia Cloud container repositories

Development tools (compiler, libraries, SDK & AI Frameworks)	CUDA toolkit & CUDA SDK PGI community edition GCC, Python, Ruby, R, Perl, Java, RAPIDs CUDA tuned Neural Network (cuDNN) Primitives TensorRT Inference Engine, DeepStream for Video analytics CUDA tuned BLAS, CUDA tuned Sparse Matrix Operations (cuSPARSE) DL Frameworks:TensorFlow,Caffe,PyTorch,Theano,Keras,caffe2,CNTK etc. ML Libraries/models & cuGraph: XGBoost,K- Means,Kalman filtering,H2O,Random Forest Installation and optimization of following OpenSource softwares : NumPy, OpenCV(Open Source Computer Vision Library), Matplotlib, Pydicom, Keras, Tensorflow, skimage, Pandas,Flask, LibROSA, Apache singa, Scikit-learn, Apache MXNe, Amazon Deep Java Library, Deeplearning4j deep learning framework, Natural Language Toolkit (NLTK), Gensim, CoreNLP, spaCy, Pytorch

PARAM Siddhi-AI Software Stack

Below diagram shows the software stack of PARAM Siddhi-AI system



1.2.2 PARAM Yuva-II

Two Subclusters	**PARAM Yuva II:**
Subcluster-1	221 nodes cluster of Intel server system R2000GZ with Dual socket Intel Xeon E5 2670 (Sandy Bridge) Processor per node Eight CPU cores per socket, 2.6 GHz Two Intel Xeon Phi 5110P per node Infiniband FDR interconnect Partitions: TESTp, FDRp, BIGJOBp, SDSp
Subcluster-2	Four nodes cluster of Supermicro SuperServer 1027GR-TRF with Dual socket Intel Xeon E5 2650 (Sandy Bridge) Processor per node Eight CPU cores per socket, 2.6 GHz Two NVIDIA GPU Tesla M2090 per node Infiniband FDR interconnect Partition: GPUp
Storage	PFS based scratch space with 10 GB/s write bandwidth User Home Area: 197TB Archival: 800TB
Software	Operating System: CentOS v6.2, Kernel v2.6.32-220 Intel Cluster Studio XE 2013 Intel Cluster Studio XE 2015 PGI Cluster Development Kit
Applications	Libraries and software for file formats, data bases and math Many scientific applications for material science/quantum chemistry, molecular modelling, computational fluid dynamics, climate modelling, circuit simulations and many more like aerospace engineering.

1.2.3 PARAM Yuva

Cluster of PARAM Yuva

PARAM Yuva:

Peak Perf. 37.8 Tflops and Rmax Perf. 54 TFlops

Networking : System Area Network (PARAM Net-3)

Speed: 10Gbps

Processor: x86 based architecture on Quad Core processors

4,608 cores of Intel Xeon 7350 processors called Tigerton

with a clock speed of 2.93 gigahertz (GHz)

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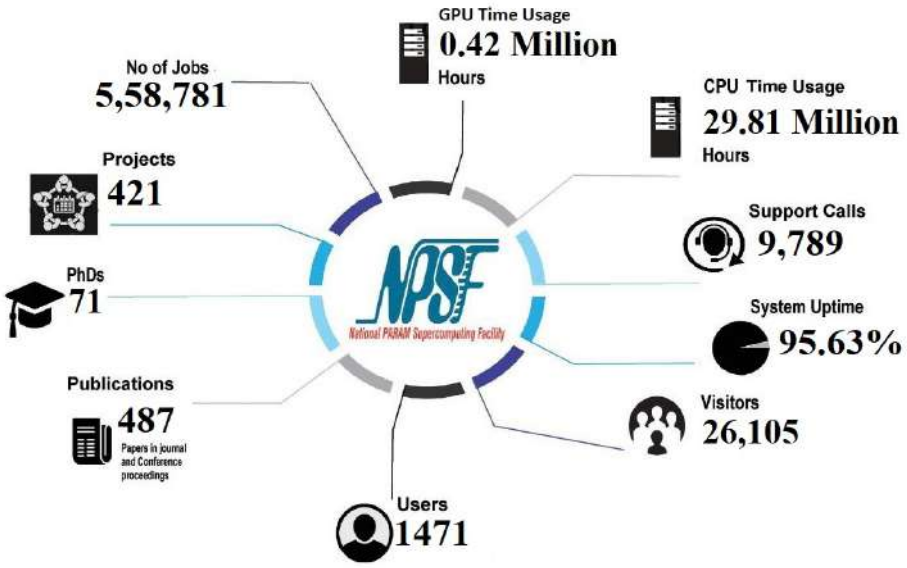
2

NPSF in Last 9 Years

Below are some of the NPSF statistics of last 9 years i.e Year 2013-2021.

The statistics includes variation in cluster utilization, year-wise total number of projects, institutes, PhDs & publications using the resources of NPSF PARAM Yuva-II and PARAM Siddhi-AI .



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2.1 Major Events

Commissioning of PARAM Siddhi-AI System in CIP DC

- Commissioning of the PARAM Siddhi-AI System in National PARAM Supercomputing Facility(NPSF) Data Center (DC), C-DAC Innovation Park(CIP) Building was carried out in phases.
- Plan was prepared with timelines and milestones for PARAM Siddhi-AI system that included verticals/phases like system architecture, deployment (physical & functional components), start of operations etc.
- Shifting of PARAM Siddhi-AI system to CIP DC: Tasks along-with timelines have been finalized and presented for shifting of PARAM Siddhi-AI system to CIP DC. The plan accounts in simultaneity in execution of tasks
- The data center is having RDHx cooled racks for hosting compute nodes and air cooled racks for hosting storage, switches, platform and periphery nodes
- Initially 28 nodes were brought from C-DAC Main Building DC to the newly commissioned NPSF, CIP DC. Rest of the 14 nodes were brought after a month time. This arrangement was made to minimize the downtime of the system and continuation of the services and support.
- Nodes were rack mounted with the help of server lift and connected with the 1GbE, 10GbE, 100 GbE and Infiniband HDR network for compute and storage.
- Commissioning of Infiniband Director Switch was carried out. It is state of the art liquid cooled director switch with 320Tb/s throughput. This was first of its kind of installation in India. All the 42 compute nodes were connected to the director switch
- Commissioning of 10.5 PiB Storage with 250 GB/sec and 4 Million 4K size Random read IOPS performance has been carried out. The storage was connected to the director switch and made available over HDR.
- System was installed, configured with Software Stack that includes HPC/ AI tools, utilities and applications for users . Access to NVIDIA GPU Cloud (NGC) is also provided.
- System S/W stack includes kubernetes for container based training /HPC workload execution, monitoring, log collection, utilization metrices, for containers, platform services (Kafka, RDBMS, ELK etc)
- System S/W stack includes Workload Manager and Scheduler (SLURM with enroot & pyxis), kubernetes for container based service deployments and other system administration related tools and services for management and monitoring of the system including C-CHAKSHU.
- HPL and GPU burn test for load test has been performed on all 42 nodes placed in CIP
- User's onboarding process was started for PARAM Siddhi-AI System in Aug-2021
- Users using the system in preview mode were migrated on the newly commissioned system (in production mode). All the users were on boarded on the system under NPSF Technical Affiliation Scheme
- Slurm workload manager (resource manager scheduler) has been introduced for preview mode users in PARAM Siddhi-AI System

- System S/W stack finalized including Kubernetes for container based training /HPC workload execution, monitoring, log collection, utilization matrices, for containers, platform services
- Work load manager Resource and Scheduler (SLURM with enroot & pyxis).
- HPL and GPU burn test for load test has been performed on all 42 nodes placed in CIP
- The 28 nodes have been commissioned along with 6 nos. of Inference and Platform nodes
- System was released in 2 stages with each stage catering to specific workload types; these are :
  I. Interim release of HPC-AI GPU infrastructure for execution of AI Training / HPC and MPI workload execution in batch mode (through SLURM) on 23 rd August 2021
  II. Release of Kubernetes cluster for model deployment for NLTM Pilot projects on 25th August, 2021(earlier slated for 29th Aug 2021)

Training

- C-DAC in collaboration with NVIDIA has organized training program for users from PARAM Siddhi-AI system.
- First part of the online 2-part training was scheduled from 15th March 2021.
- Training program had notable HPC-AI experts delivering talks ranging from CUDA computing, NVIDIA A100 GPU, various AI tools to demo and hands-on on applications on GPU.
- The purpose of 2 stages training program was to hear out ideas, take feedback from participants, and with that, comprehend future training and workshop requirements to further evolve detailed deep dive training program for execution in 2nd stage.
- It was with the intent that the said training program will set the stage for usage of converged HPC-AI infrastructure by researchers, students and Start-ups alike and foster a community encircling PARAM Siddhi-AI at the core.

Bootcamps and Hackathons

1) OpenACC Bootcamp Phase 1

OpenAcc BootCamp was organized in collaboration with NVIDIA on 17th Feb, 2021. The event was conducted online. 56 participants were on-boarded on the system and 8 nos. of NVIDIA DGX-A100 systems were used. Environment setup, and round the clock support was provided by NPSF Help team. Link: https://www.gpuhackathons.org/event/c-dac-india-gpu-bootcamp

2) OpenACC Bootcamp Phase 2

OpenACC Bootcamp Phase 2 was conducted on 23rd Feb, 2021. By enabling MIG feature of the A100 GPUs, we have provided the GPU instances to the participants and we could accommodate 81 participants on 2 DGX-A100 nodes. This otherwise would have required 11 compute nodes. 81 participants were on-boarded on the system. . Environment setup, and round the clock support was provided by NPSF Help team. Link: https://www.gpuhackathons.org/event/c-dac-india-gpu-bootcamp

3) AI For Science Bootcamp

AI for Science Bootcamp was targeted towards learning how AI can accelerate HPC simulations by introducing the concepts of Neural Networks, including data pre-processing, and techniques on how to build, compare and improve accuracy of models Enabling. We have provided the GPU instances to the participants and we could accommodate 84 participants on 4 DGX-A100 nodes. Environment setup, user on boarding. Preparation of System usage manual for the bootcamp. 84 participants have been on-boarded on the system. Environment setup, and round the clock support was provided by NPSF Help team. Link: https://www.gpuhackathons.org/event/c-dac-ai-science-bootcamp

4) GPU Application Hackathon / C-DAC HPC Hackathon

GPU Application Hackathon 2021 was arranged in collaboration with NVIDIA and it continued till 4th August 2021. 61 users were on-boarded for using PARAM Siddhi-AI system. Required tools were installed, demo was to the participants and manual was circulated. The access to the nodes was provided through scheduler and support was provided through SLACK Link: https://www.gpuhackathons.org/event/c-dac-hpc-hackathon-2021

PARAM Siddhi-AI System Downtime

- PARAM Siddhi-AI system services were interrupted due to failure in the electrical infrastructure on 2nd Sep, 2021. The downtime lasted for 151:32 Hours.
- Access to PARAM Siddhi-AI system and interactive batch job submission was interrupted due to planned maintenance activity on login node on 29th Sep, 2021. The downtime lasted for 2 hours.
- Access to PARAM Siddhi-AI system was interrupted due to planned network maintenance activity in NOCC on 22nd Oct, 2021. The downtime lasted for 2.25 hours
- PARAM Siddhi-AI system services were interrupted due to issue with the cooling infrastructure of the Infiniband Director Switch on 25th Dec, 2021. The downtime lasted for 113:24 Hours.

PARAM Yuva-II:

- We continued to serve NPSF user community who have access to PARAM Yuva-II system
- As an effort to apprise Chief Investigators (CI) of projects in NPSF, and also to serve as usage charges levied (not commercial), NPSF has been raising invoices for monthly CPU time utilization. In 2021, total 1884 invoices have been raised against consumed CPU Time of 29815250 CPU Hours. The e-money equivalent of the consumed CPU Time is 29815.25 debit units.

Acknowledgement

The activities of the National PARAM Supercomputing Facility were supported by the grant-in-aid financial support from MeitY, Ministry of Electronics and Information Technology, under the National Supercomputing Mision(NSM). We gratefully acknowledge the funding of these projects by MeitY,

2.2 Statistics

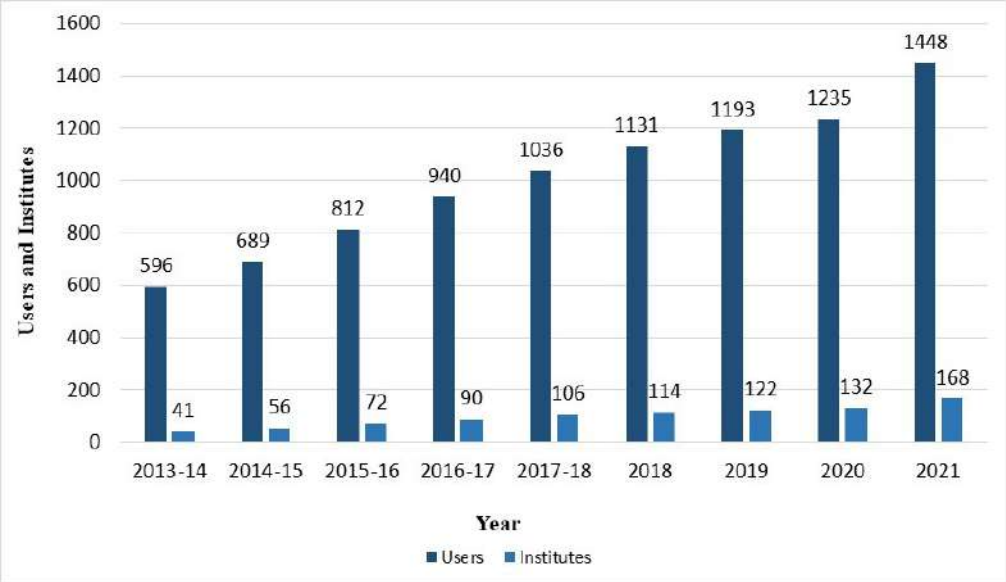

Figure: Year wise Total Users and Institutes

Table: Year wise total users and institutions

Year	Users	Institutes
2013-14	596	41
2014-15	689	56
2015-16	812	72
2016-17	940	90
2017-18	1036	106
2018	1131	114
2019	1193	122
2020	1235	132
2021	1448	168

The above bar graph shows growth in the count of NPSF PARAM Yuva-II and PARAM Siddhi-AI **Users and Institutes** under the NPSF Technical Affiliation Scheme(TAS). Notably, the number of users has doubled, and the number of institutions has tripled in the last 9 years.

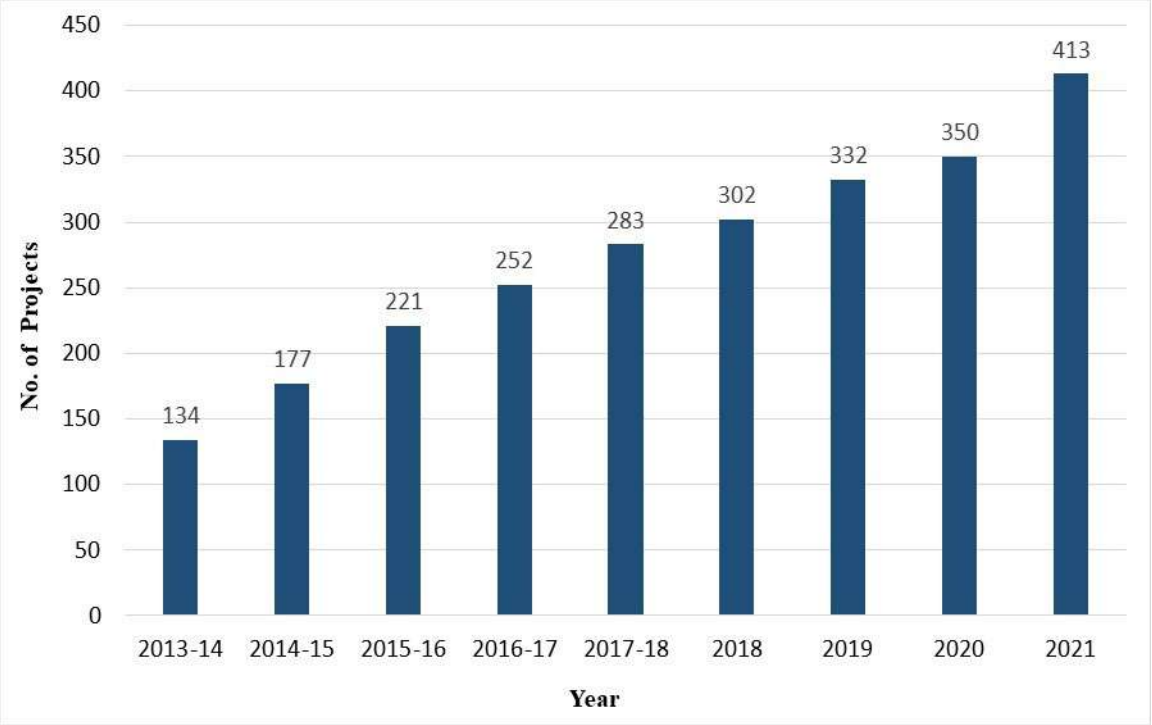

Figure: Year wise Total Number of Projects

Table: Year wise total number of projects

Year	Number of Projects
2013-14	134
2014-15	177
2015-16	221
2016-17	252
2017-18	283
2018	302
2019	332
2020	350
2021	413

The above bar graph shows the substantial growth in the **Number of Projects** registered with NPSF in the last 9 years; worth to mention the addition of PARAM Siddhi-AI projects too.

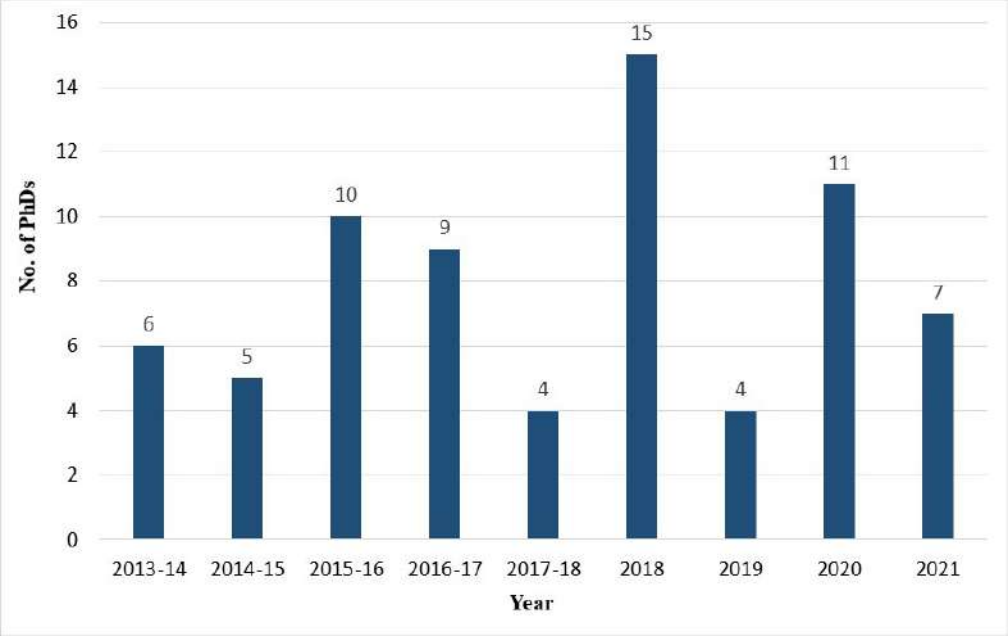

Figure: Year wise Total Number of PhDs

Table: Year wise Total number of PhDs

Year	**Number of PhDs**
2013-14	6
2014-15	5
2015-16	10
2016-17	9
2017-18	4
2018	15
2019	4
2020	11
2021	7

The above graph shows the **Count of PhDs** completed using the resources of NPSF PARAM Yuva-II and PARAM Siddhi-AI systems. In the last 9 years, total 71 PhDs have been completed. In 2021, 6 PhDs awarded using the resources of PARAM Yuva-II and 1 using the GPU resources of PARAM Siddhi-AI system.

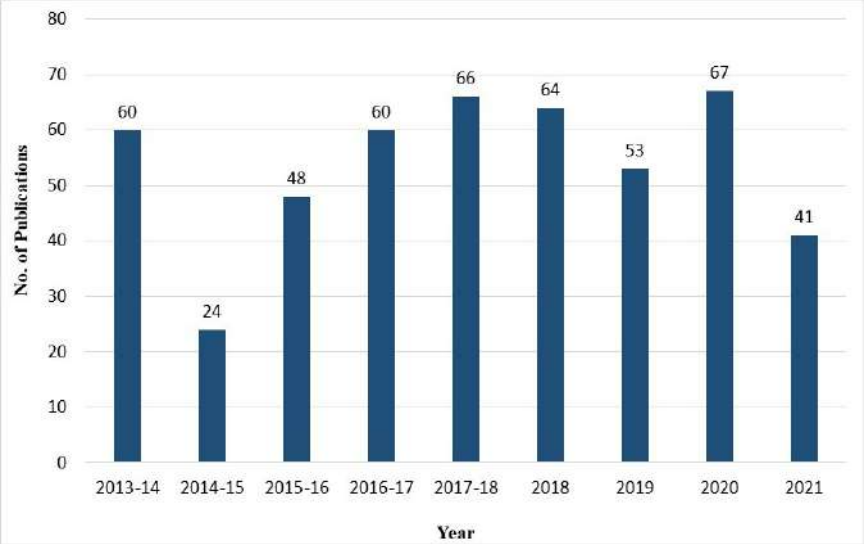

Figure: Year wise Total Number of Publications

Table: Year wise Total number of publications

Year	**Number of Publications**
2013-14	60
2014-15	24
2015-16	48
2016-17	60
2017-18	66
2018	64
2019	53
2020	67
2021	41

NPSF users publish their research work in reputed journals and conferences where they acknowledge the NPSF PARAM Yuva- II and PARAM Siddhi-AI . The above graph shows the **Total Number of Publications** using both the systems of NPSF, which is 487 In the last 9 years. Whereas, In 2021, 35 publications were reported using PARAM Yuva-II and 6 publications using PARAM Siddhi-AI.

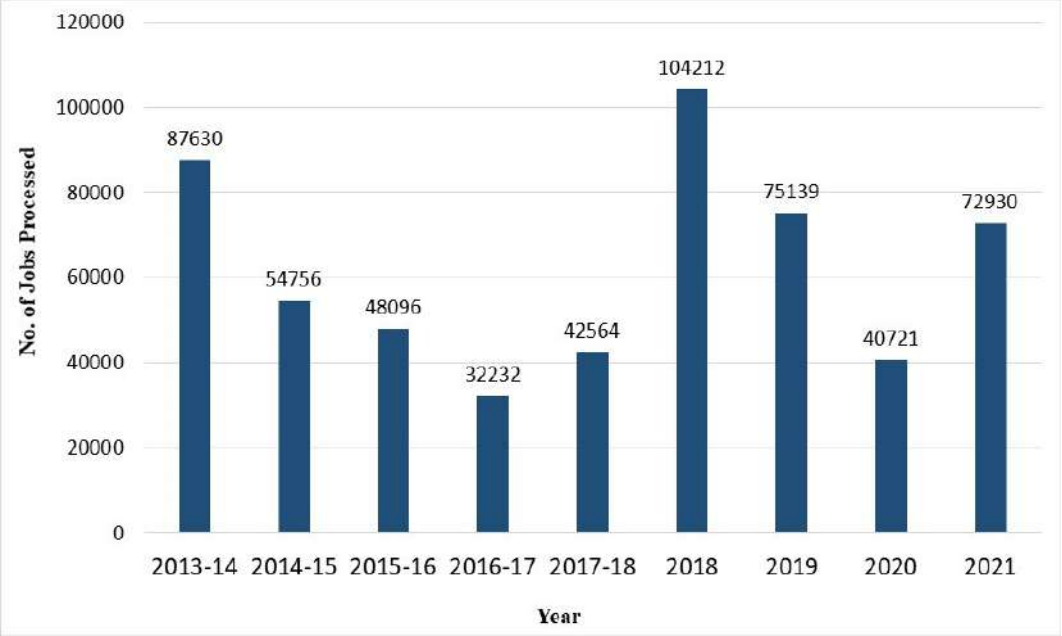

Figure: Year wise Total Number of Jobs Processed

Table: Year wise Total number of jobs processed

Year	**Number of jobs processed**
2013-14	87630
2014-15	54756
2015-16	48096
2016-17	32232
2017-18	42564
2018	104212
2019	75139
2020	40721
2021	72930

The above graph shows the **Total Number of Jobs Processed** using NPSF PARAM Yuva-II and PARAM Siddhi-AI systems, which has been more than 5.5 Lakh in the last 9 years. Notably, in 2021, inspite of system unavailability (planned and unplanned downtime) of 5.66 % of both the systems, the count of the jobs processed is close to 73 thousand.

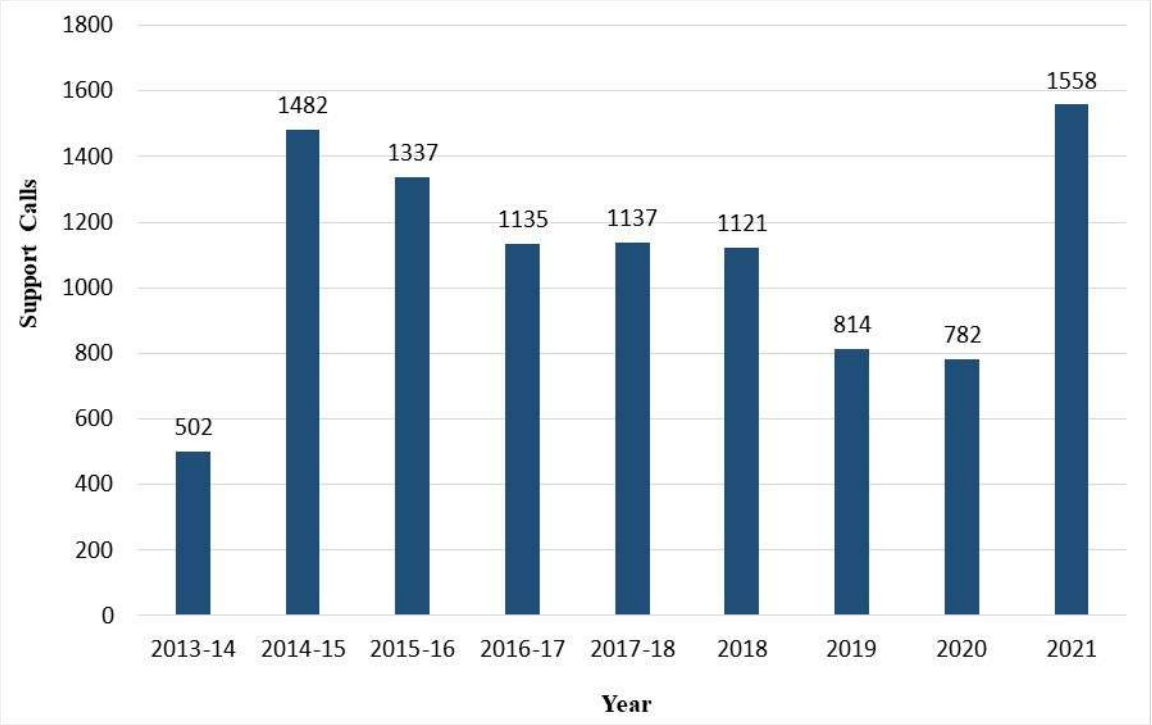

Figure: Year wise Total Number of Support Calls

Table: Year wise Total number of support calls

Year	Number of support Calls
2013-14	502
2014-15	1482
2015-16	1337
2016-17	1135
2017-18	1137
2018	1121
2019	814
2020	782
2021	1558

The above bar graph shows **Year wise Number of Support Calls** raised by NPSF users and addressed by NPSF team. Users generally require technical support while on-boarding the system and, after that, for using the system. Around 9789 support calls were handled till 2021 via group video conferencing (using C-DAC's in-house developed video conferencing plateform - Sangoshthee), telephonic discussion, and e-mail, which also includes the count of support calls right from the release of the PARAM Siddhi-AI system in preview mode.

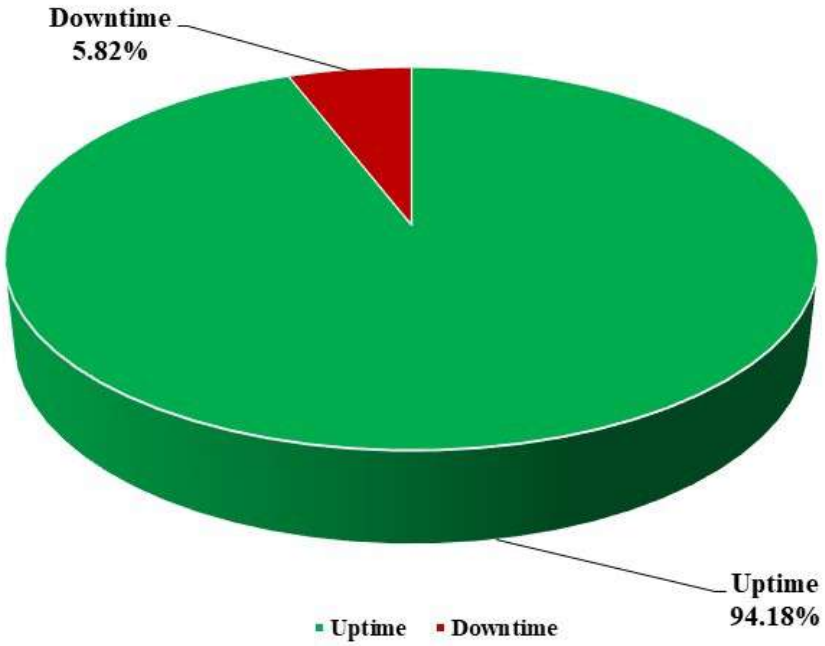

Figure: 9 years System Availability(Cumulative of PARAM Yuva-II & PARAM Siddhi-AI)

Table: 9 Years System availability

Year	Uptime(%)	Downtime(%)
2013-14	93	7
2014-15	91.6	8.36
2015-16	97	3
2016-17	99.2	0.8
2017-18	99.17	0.83
2018	99.95	0.05
2019	70.31	29.69
2020	98.92	1.08
2021	94.18	5.82

One of the most important aspects of any HPC facility is the system's availability. NPSF system has 94.34% of the uptime over the last 9 years, which is cumulative of PARAM Yuva-II and PARAM Siddhi-AI systems, whereas the system's downtime was reported as only 5.66%.

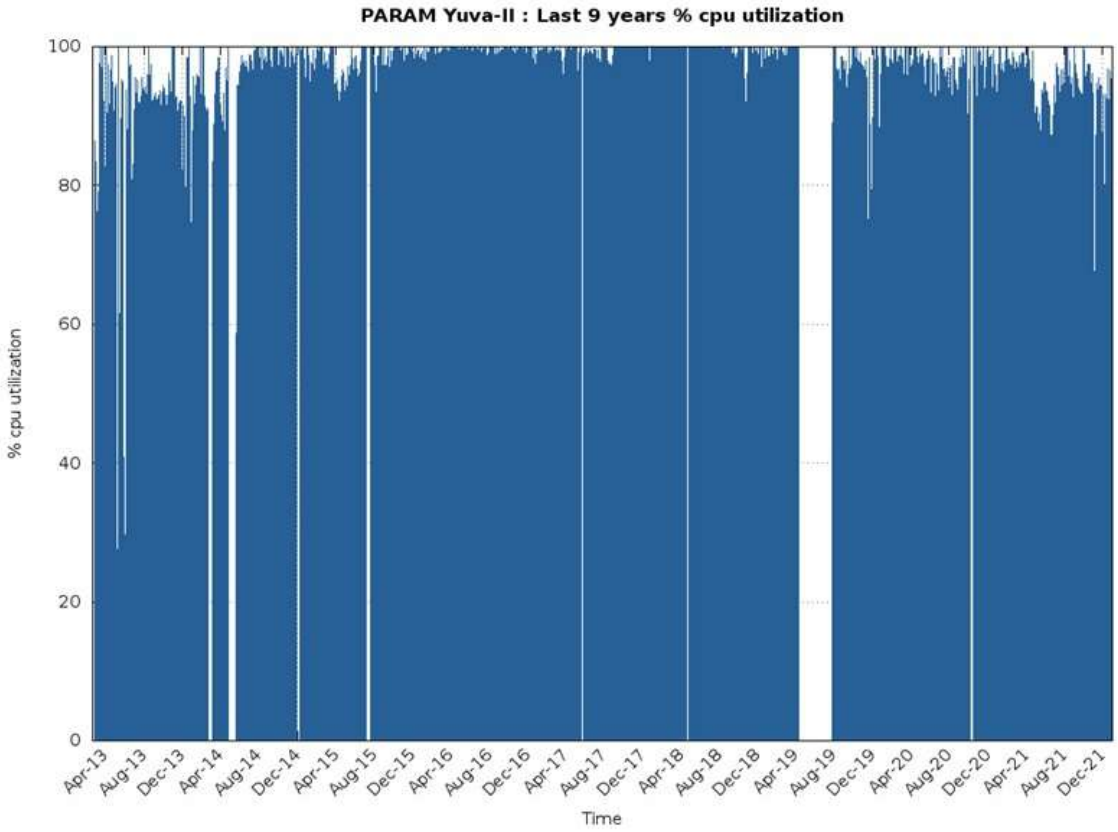

Figure: CPU Utilisation in 9 Years

In the HPC system, % CPU utilization is calculated as % of CPU cores used out of available CPU core. NPSF team monitors the CPU usage, which records every minute in the database. The above GNU Plot shows the **Utilization of CPU cores** above 90% most of the time in the last 9 years. This graph also presents the high utilization of the system consistently.

3

Statistics of PARAM Siddhi-AI

3.1 System

System Availability

The below pie chart represents the PARAM Siddhi-AI system's availability by showing the statistics of uptime as 96.93 % and downtime as 3.07%. NPSF PARAM Siddhi-AI downtime was reported from planned (0.05%) and unplanned (3.02%) aspects. PARAM Siddhi-AI system services were interrupted due to failure in the electrical infrastructure on 2nd Sep, 2021. The downtime lasted for 151:32 Hours. Access to PARAM Siddhi-AI system and interactive batch job submission was interrupted due to planned maintenance activity on login node on 29th Sep, 2021. The downtime lasted for 2 hours. Access to PARAM Siddhi-AI system was interrupted due to planned network maintenance activity in NOCC on 22nd Oct, 2021. The downtime lasted for 2.25 hours. PARAM Siddhi-AI system services were interrupted due to issue with the cooling infrastructure of the Infiniband Director Switch on 25th Dec, 2021. These failures have impacted the overall availability of the PARAM Siddhi-AI system and services to the users.

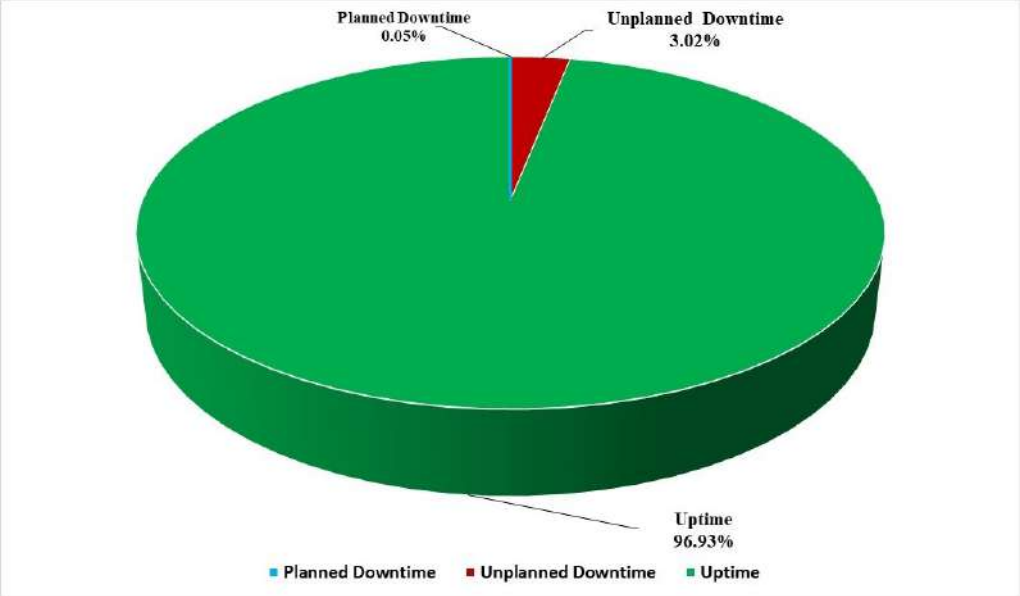

Figure: PARAM Siddhi-AI System Availability

Table: PARAM Siddhi-AI System Availability

Uptime %	Planned downtime %	Unplanned downtime %
96.93	0.05	3.02

System utilization

The above GNU plot shows the PARAM Siddhi-AI system utilization. NVIDIA A100 GPU is the core component of PARAM Siddhi-AI system, where % GPU utilization is calculated as % of GPU used by the users in batch jobs for computation, out of the total available number of GPU, as indicated by the scheduler. This GPU utilization is recorded every minute in the database. From the GNU plot, It can be seen that most of the time, system utilization remained above 90% throughout the year. The gaps in the plot are indicative of the non-availability of the system and few times, the non-availability of the data.

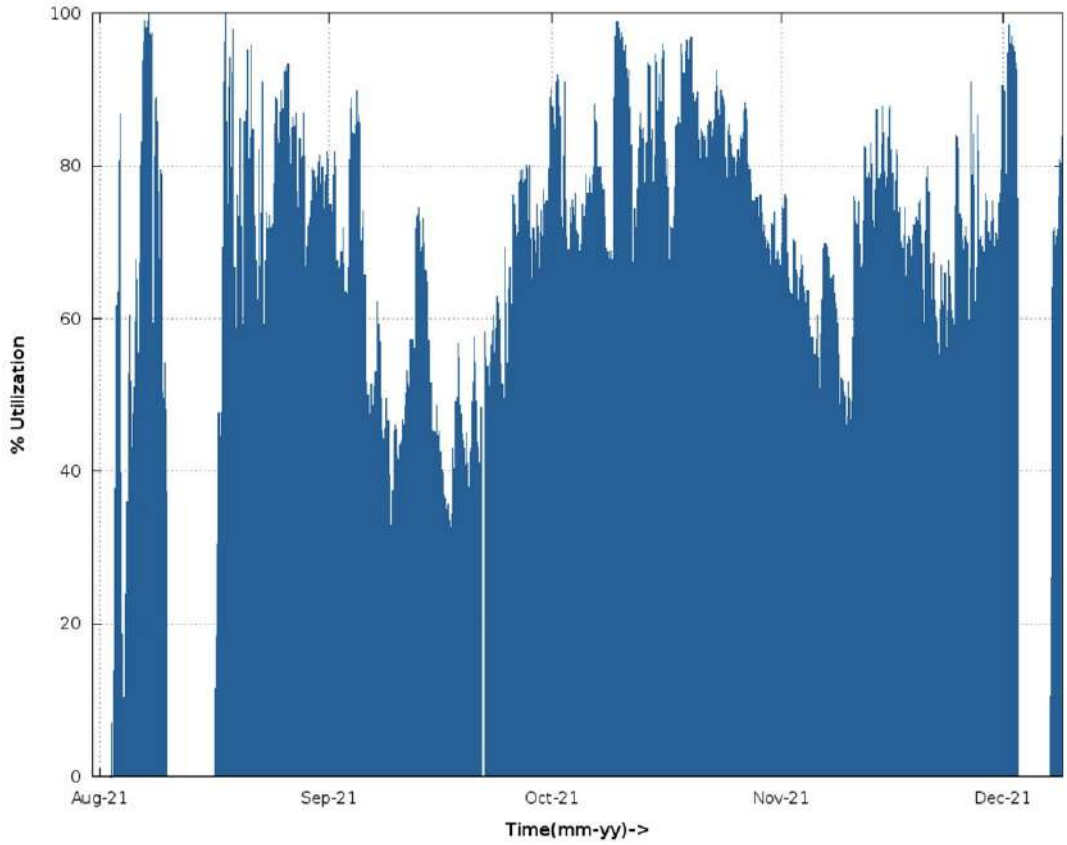

Figure: PARAM Siddhi-AI System Utilisation

GPU time utilization w.r.t. No. of GPUs

The graph below shows the GPU time utilization as per the different job sizes of NVIDIA GPU A100. The Job size 5-12 has the maximum utilisation of GPUs followed by the job sizes 1-4 and 13-28 respectively .

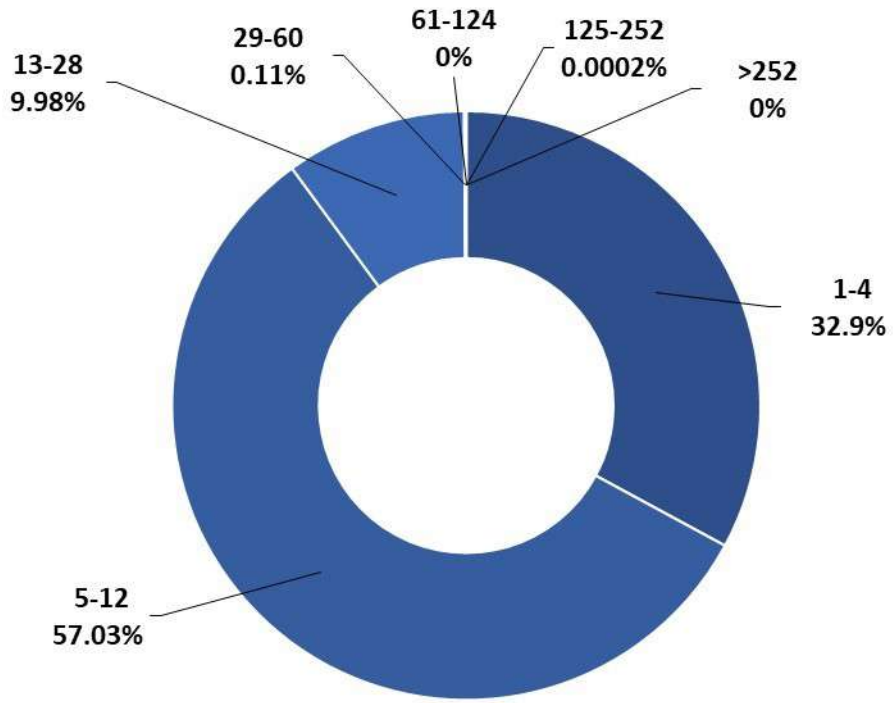

Figure: PARAM Siddhi-AI GPU Time Utilisation w.r.t. Job Sizes

Table: GPU time utilization w.r.t. No. of GPUs

No. of GPUs	GPU Hours
1-4	139728
5-12	242487
13-28	42469.1
29-60	499.64
61-124	0
125-252	0.912
>252	0

% distribution of jobs w.r.t. Job Size(No. of GPUs)

Below donut shows the distribution of Jobs w.r.t job sizes, where job sizes are distributed in the range of 1-4 GPUs, 5-12 GPUs, 13-28 GPUs, 29-60 GPUs, 61-124 GPUs , 125-252 GPUs and >252 GPUs.

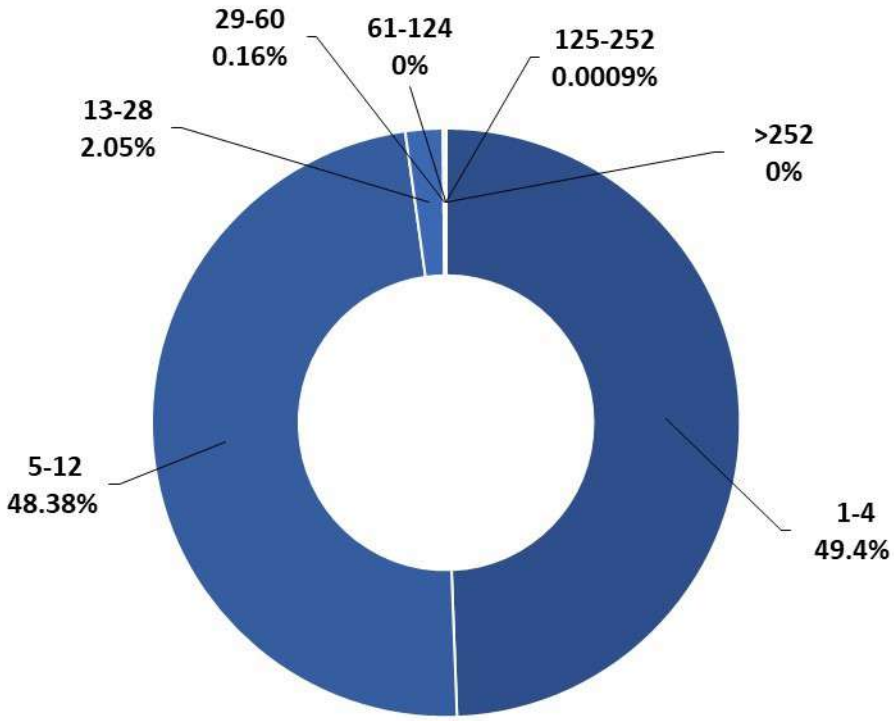

Figure: Distribution of Jobs as per the Job Sizes (No. of GPUs)

Table: % distribution of jobs w.r.t. Job Size(No. of GPUs)

No. of GPUs	Job Count
1-4	5890
5-12	5769
13-28	244
29-60	20
61-124	0
125-252	1
>252	0

Absolute wait time Vs no. of jobs

Absolute wait time for a job is the time spent in the queue, after submission, till allocation of resources and execution. The graph below shows that the maximum number of jobs do not have to wait longer than 0.05 hours, which shows the higher availability of PARAM Siddhi-AI resources.

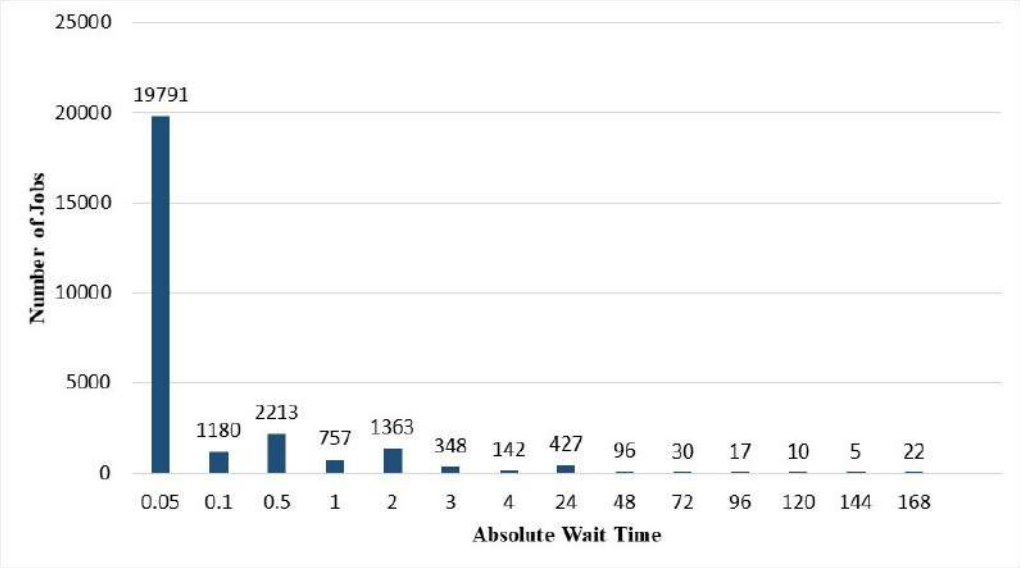

Figure: Absolute wait time Vs. No. of Jobs

Table: Absolute wait time Vs no. of jobs

Absolute wait Time(in hours)	Number of Jobs
0.05	19791
0.1	1180
0.5	2213
1	757
2	1363
3	348
4	142
24	427
48	96
72	30
96	17
120	10
144	5
168	22

Execution time Vs Number of Jobs

The above graph represents the execution time of the jobs in hours. It is noticeable that only 1.03% of the total jobs were executed for 7 days which is the maximum limit of the wall time of the jobs. Whereas a large number of jobs, 19386 executed within 0.1 hours.

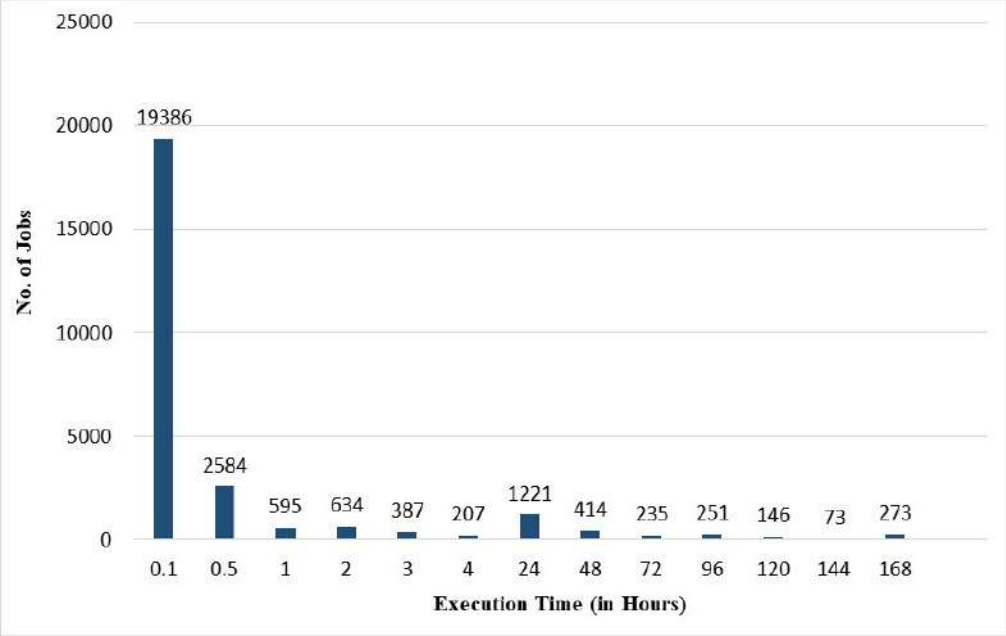

Figure: Execution Time Vs No. of Jobs

Table: Execution time Vs Number of Jobs

Execution time(in hours)	**Number of Jobs**
0.1	19386
0.5	2584
1	595
2	634
3	387
4	207
24	1221
48	414
72	235
96	251
120	146
144	73
168	273

Relative measure of job wait time with respect to its execution time, binned by job size

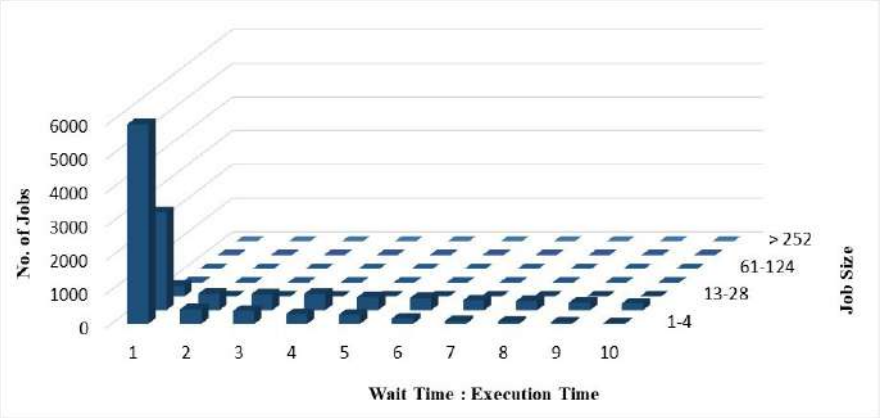

Figure: Relative measure of job wait time with respect to its execution time, binned by job size

Table: Ratio of job waittime: execution time Vs number of jobs

GPU/Ratio	1	2	3	4	5	6	7	8	9	10
1-4	5920	435	388	291	276	163	84	70	49	29
5-12	2900	487	472	483	384	364	291	271	228	201
13-28	316	7	5	0	0	0	0	0	0	0
29-60	10	0	0	0	0	0	0	0	0	0
61-124	0	0	0	0	0	0	0	0	0	0
125-252	1	0	0	0	0	0	0	0	0	0
>252	0	0	0	0	0	0	0	0	0	0

User Support Calls

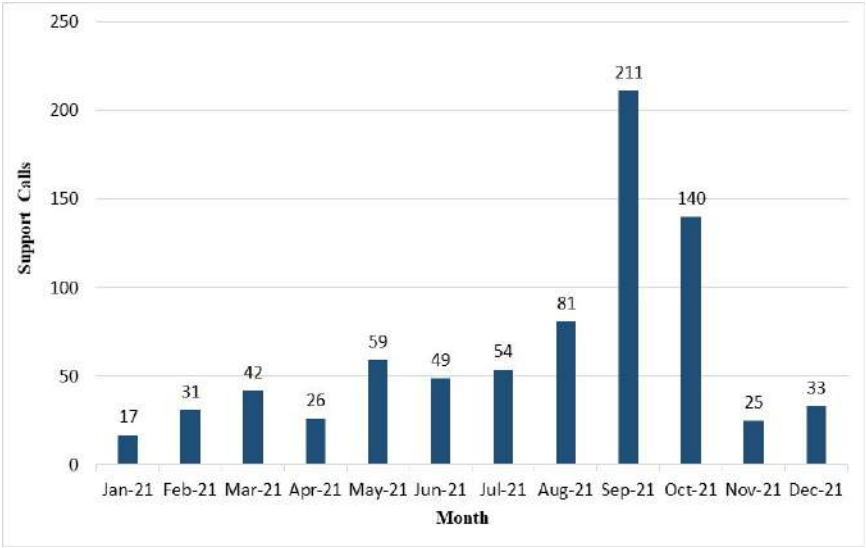

Figure: Monthwise User Support Calls 2021

Above graph indicates distribution of month wise number of support calls in 2021. It also includes the count of PARAM Siddhi-AI support calls from the release in preview mode.

Table: Month Wise Number of Support Calls 2021

Month	Number of Support Calls
Jan-2021	17
Feb-2021	31
Mar-2021	42
Apr-2021	26
May-2021	59
Jun-2021	49
Jul-2021	54
Aug-2021	81
Sep-2021	211
Oct-2021	140
Nov-2021	25
Dec-2021	33

3.2 Users and Institutes

Institute wise GPU time utilization

User Jobs running over the cluster consume the GPU Time of the cluster. Above doughnut, plot represents the % distribution of GPU Time consumed by the Research Organizations/Academic Institutes. As seen in the 2021 plots, Jobs submitted from users of IIT Madras continuously consume the max. % of GPU Time.

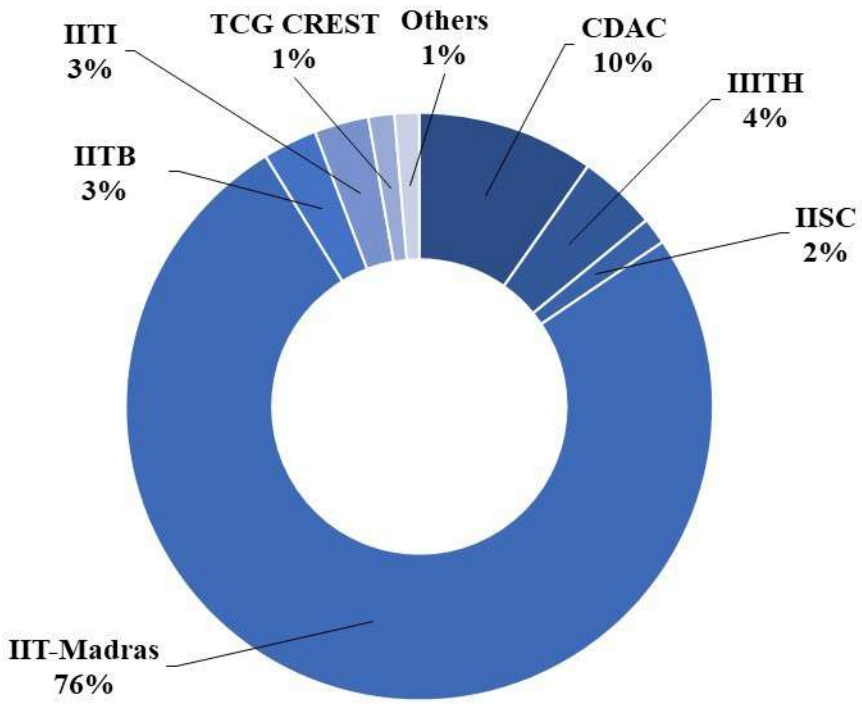

Figure: Institute % wise GPU time utilization

Table : Institute wise GPU time utilization Year-2021

Code	Institute Name	GPU Time Utilization(in Hours)
CDAC	Centre for Development of Advanced Computing	1123
DIAT	Defence Institute of Advanced Technology	15
ICAR	Indian Council of Agricultural Research	16
IIITH	Indian Institute of Information Technlogy, Hyderaabad	499
IISC	Indian Institute of Science, Bangaluru	169
IITD	Indian Institute of Technology, Delhi	9
IITK	Indian Institute of Technology, Kanpur	86
IIT-Madras	Indian Institute of Technology, Madras	8724
IITB	Indian Institute of Technology, Bombay	345
IITI	Indian Institute of Technology, Indore	345
TCG CREST	Centres for Research and Education in Science and Technology, Kolkata	164
IITBBS	Indian Institute of Technology, Bhubaneswar	31

Institute and job size(No. of GPU) wise job count

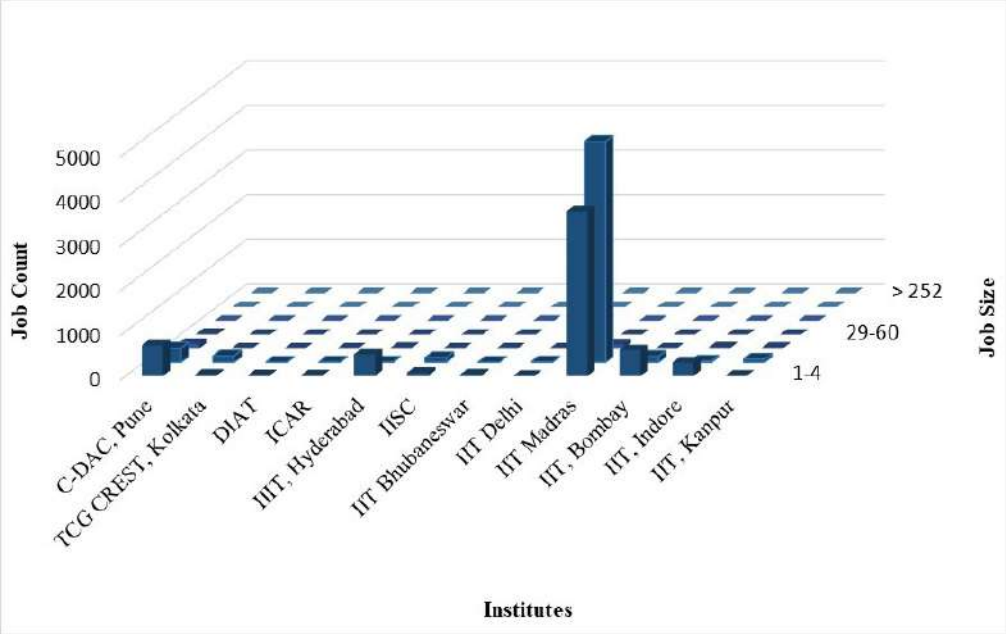

Figure: Institute and job size(No. of GPU) wise job count

Table : Institute and Job size wise Job count(2021)

Code	Institute Name	1-4	5-12	13-28	29-60	61-124	125-252	>252
CDAC	Centre for Development of Advanced Computing	686	316	104	17	0	0	0
TGC-CREST, Kolkata	Centres for Research and Education in Science and Technology	27	137	0 0	0 0	0 0	0 0	0 0
DIAT	Defence Institute of Advanced Technology	15	0	0	0	0	0	0
IISC	Indian Institute of Science, Bangaluru	69	100	0	0	0	0	0
IITBBS	Indian Institute of Technology,Bhubaneswar	31	0	0	0	0	0	0
IITD	Indian Institute of Technology, Delhi	2	7	0	0	0	0	0
IITM	Indian Institute of Technology, Madras	3686	4949	87	1	0	1	0
IITB	Indian Institute of Technology, Bombay	577	128	0	0	0	0	0
IITI	Indian Institute of Technology, Indore	297	26	22	0	0	0	0
IITK	Indian Institute of Technology, Kanpur	4	66	16	0	0	0	0

Number of publications across institutes

User's Research work resulted in Publications; below doughnut plot represents the % wise publications across Research Organizations/Academic Institutes. In the Year 2021 total of 6 Research Paper has been published using PARAM Siddhi-AI cluster.

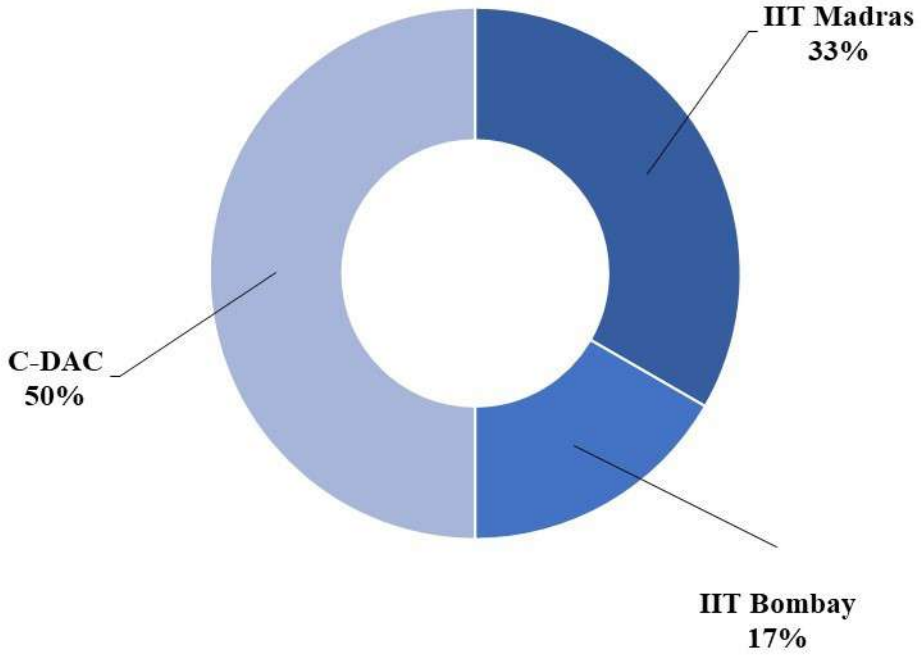

Figure: Number of publications across institutes 2020

Table: Number of publications across research institutes-2021

Institute	**Number of Publications**
IIT Madras	2
Indian Institute of Technology Bombay	1
C-DAC	3

Number of PhDs across institutes

One PhD was awarded to Pruthwik Mishra from IIIT, Hyderabad under the supervision of Prof Dipti Misra Sharma. His research work includes Infrastructure for "IIITH MT systems" and running "Bahu-bhashak" (NLTM) in the research area of AI/ML/DL.

Table : State wise PARAM Siddhi-AI users and Institutes

State or Union Territory	Short Name	No. of Institutions	No. of Users
West Bengal	WB	1	8
Bihar	BR	1	2
Delhi	DL	6	11
Gujarat	GJ	1	1
Karnataka	KA	3	28
Kerela	KL	2	7
Madhya Pradesh	MP	1	10
Maharashtra	MH	3	53
Odisha	OD	1	2
Tamil Nadu	TN	1	32
Telangana	TS	2	6
Uttar Pradesh	UP	2	6

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Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawnto scale nor conforms to international/ state borders in its entirety.

Table : State wise PARAM Siddhi-AI Job processsed

State or Union Territory	**Short Name**	**No. of Jobs**
Delhi	DL	101
Karnataka	KA	260
Kerela	KL	24
Maharashtra	MH	2898
Odisha	OD	52
Tamil Nadu	TN	20816
Uttar Pradesh	UP	120
West Bengal	WB	254

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Jobs Processed

Jobs Processed in %

Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawnto scale nor conforms to international/ state borders in its entirety.

Table : State wise PARAM Siddhi-AI Job processsed

State or Union Territory	Short Name	Number of Active Projects
Bihar	BR	1
Delhi	DL	5
Gujarat	GJ	1
Karnataka	KA	7
Kerela	KL	1
Madhya Pradesh	MP	3
Maharashtra	MH	29
Odisha	OD	1
Tamil Nadu	TN	3
Telangana	TS	2
Uttar Pradesh	UP	3
West Bengal	WB	1

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Projects

Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawnto scale nor conforms to international/ state borders in its entirety.

Table : State wise GPU time utilization

State or Union Territory	**Short Name**	**GPU Time(In GPU hours)**
Delhi	DL	96687
Karnataka	KA	2769515
Kerela	KL	4626
Madhya Pradesh	MP	134538
Maharashtra	MH	10137464
Odisha	OD	10315
Tamil Nadu	TN	30078453
Telangana	TS	3539603
Uttar Pradesh	UP	29584
West Bengal	WB	749333

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GPU Time Utilization in %

Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawnto scale nor conforms to international/ state borders in its entirety.

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3.3 Domain & Sectoral Usage

Users, when affiliated with NPSF are classified according to their 1) Research Field and 2) Institute. Institute is one of the attributes of the Technical Affiliation Scheme (TAS) form. This section presents GPU time distribution, job count, and job size distribution across various Research Fields and Institutes. The inferences that can be derived from this data are to assess and corroborate the percolation of HPC across application Research Fields and Institutes. Also, an assessment towards determining perpetual usage. Below list shows the list of PARAM Siddhi-AI application research fields :

Table: List of application research fields on NPSF

S.No.	Research Fields
1	Conversational AI
2	Computer Vsion
3	Cognitive Computing
4	Astronomy & Astrophysics
5	Atomic & molecular Science
6	Bio Science
7	Bioinformatics
8	Chemical Science
9	Climate & Environmental Science
10	Complex System & Statistical Physics
11	Computational Fluid Dynamics
12	Computational Physics
13	Computational Science
14	Big Data Analytics
15	Geological Science
16	Material Science
17	Quantum Mechanics
18	Structural Engineering Mechanics
19	Uncotegorised

Application Research Field Vs GPU time utilization

Below doughnut represents the % GPU Time utilization across application research fields. Conversational-AI has the highest usage of GPU time utilization which includes the variety of applications such as Automatic Speech Recognition(ASR), Text-to-Speech(TTS), Natural Language Processing(NLP) followed by Atomic & Molecular Physics.

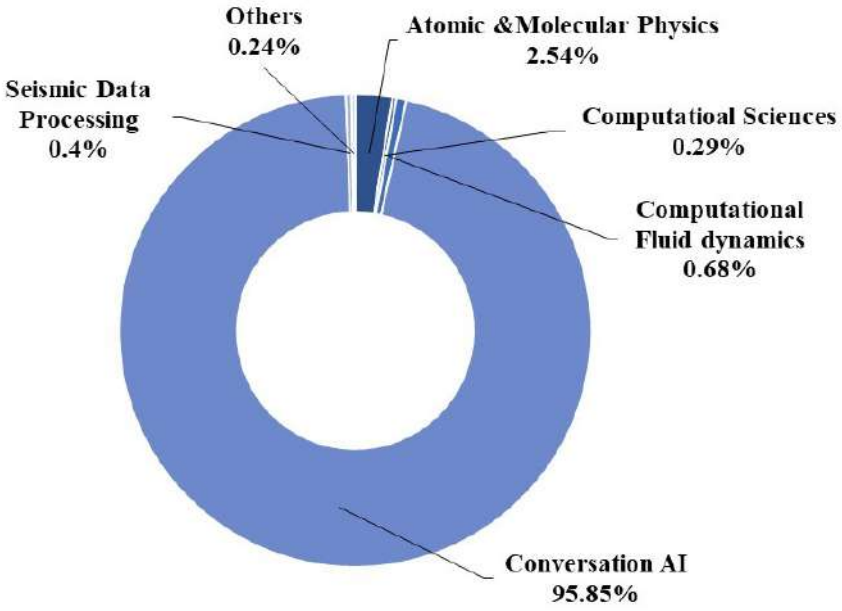


Figure: Research Field wise GPU time utilization

Table: Research Field wise GPU time utilization

Application Research Field	**GPU Hours**
Atomic & Molecular Physics	21674.03
Bioinformatics	1685.17
Computatioal Sciences	2510.27
Computational Fluid dynamics	5797.48
Computer Vision	2.3
Conversational AI	817710.55
Environmental Science	8.2
Material Science	409.13
Seismic Data Processing	3258.3

Job distribution across application research fields

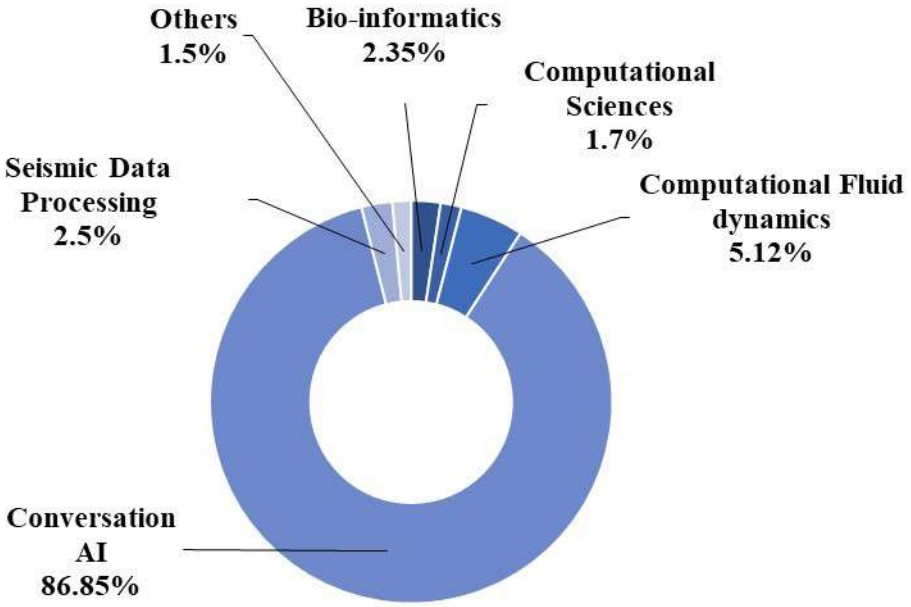


Figure: Job distribution across application research fields

Above plots shows application research fields wise percentage distribution of number of jobs processed.

Table: Job distribution across application research fields

Application Research Field	No. of Jobs
Atomic&Molecular physiscs	196
Bio-informatics	455
Computational Sciences	325
Computational Fluid dynamics	989
Computer Vision	9
Conversation AI	16777
Environmental Science	9
Material Science	76
Seismic Data Processing	479

Job sizes across application research fields

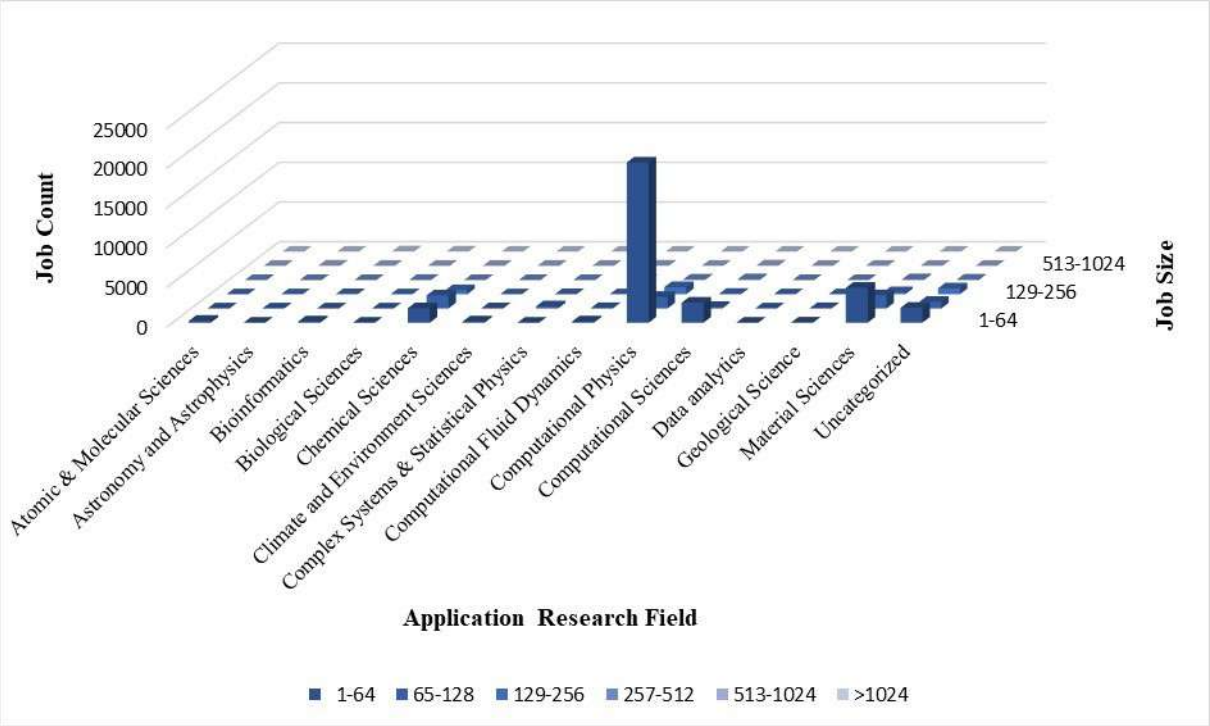


Figure: Job sizes across application research fields

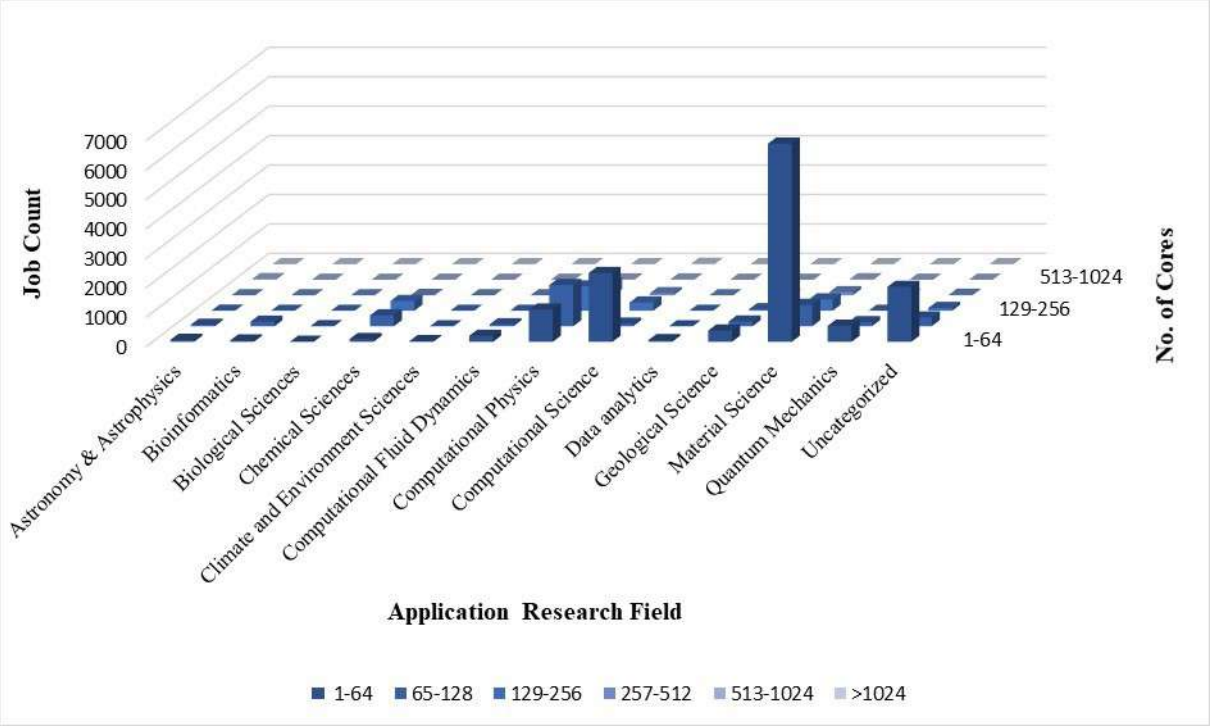


Figure: Job sizes across application research fields

Above plots depicts distribution of jobs in reference to number of GPUs requested, binned by ranges 1,2,3,4,8,16,32,64 & above.

Table: Number of Jobs and Job Sizes across Application Research Fields 2021

Application Research Fields	1-4	5-12	13-28	29-60	61-124	125-252	>252
Atomic & Molecular Physics	27	169	0	0	0	0	0
Bioinformatics	404	28	23	0	0	0	0
Computational Sciences	273	50	2	0	0	0	0
Computational Fluid Dynamics	877	86	26	0	0	0	0
Computer Vision	2	7	0	0	0	0	0
Conversational AI	6548	10007	213	8	0	1	0
Environmental Science	9	0	0	0	0	0	0
Material Science	74	2	0	0	0	0	0
Seismic Data Processing	250	145	80	4	0	0	0

AI Benchmark Model vs. Distribution of Workloads

Below doughnut plot represents the AI Benchmark Model vs. Distribution of Workloads .

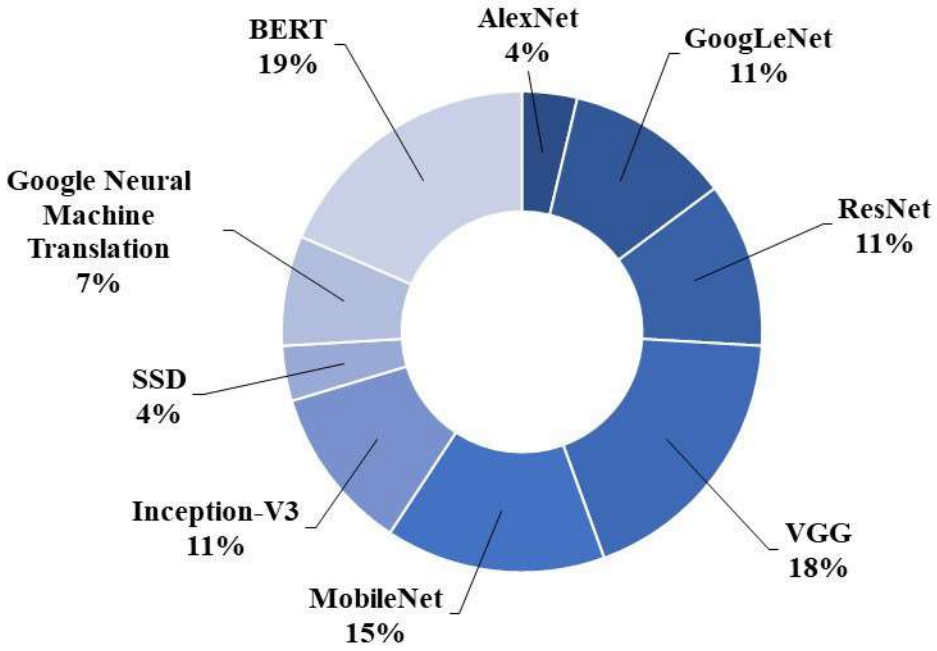


Figure: AI Benchmark Model vs. Distribution of Workloads

Table: AI Benchmark Model vs. No. of Workloads

AI Benchmark Model	No. of Workloads
AlexNet	1
GoogLeNet	3
ResNet	3
VGG	5
MobileNet	4
Inception-V3	3
BERT	5
Google Neural Machine Translation(GNMT)	2
SSD	1

Sectoral Usage vs. Distribution of projects(2021)

Sectoral usage is considered as special attention and benefit to the particular sector due to execution of the project . Ministry of Electronics & IT(MeiTY) has listed the 17 potential key sectors , these are :

- Agriculture
- Food
- Health
- Water Resource
- Environment and Pollution
- Education
- Culture
- Specially Abled
- Transportation
- Highways and Waterways
- Railway
- Energy
- Habitat
- Public Safety
- Disaster Management
- Legal
- Finance

Below doughnut represents the Sectoral Usage wise distribution of projects .

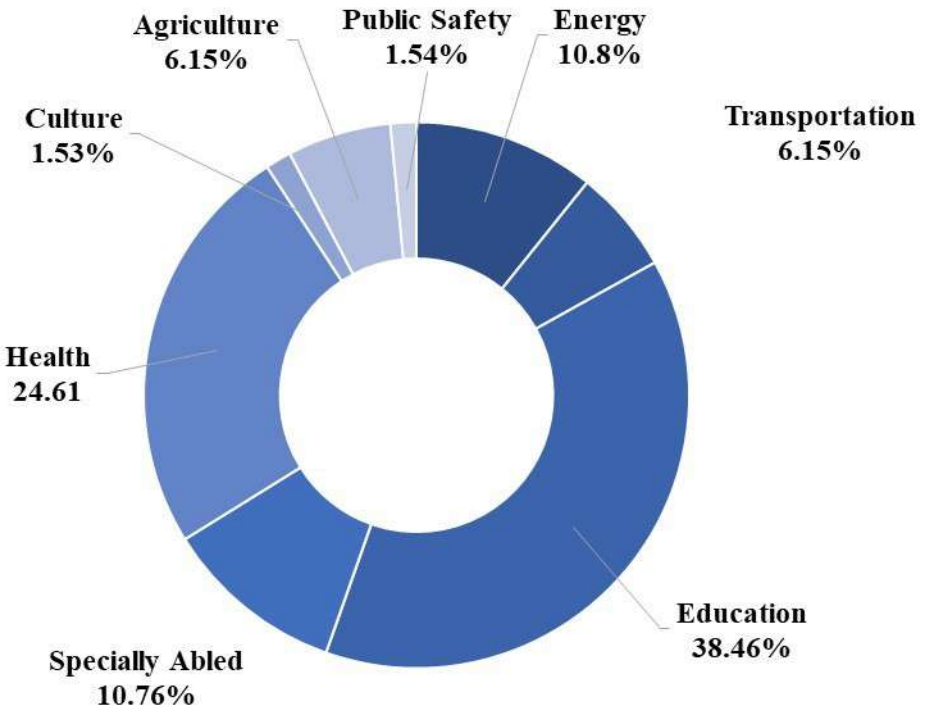


Figure: Sectoral Usage wise distribution of projects

Table: Sectoral Usage wise distribution of projects

Key Sectors	**No. of Projects**
Energy	7
Transportation	4
Education	25
Specially Abled	7
Health	16
Culture	1
Agriculture	4
Public Safety	1

Number of publications across research fields

Below doughnut plot represents the % number of Publications across Application Research field. Majority of the Publications belongs to Computational Fluid Dynamics.

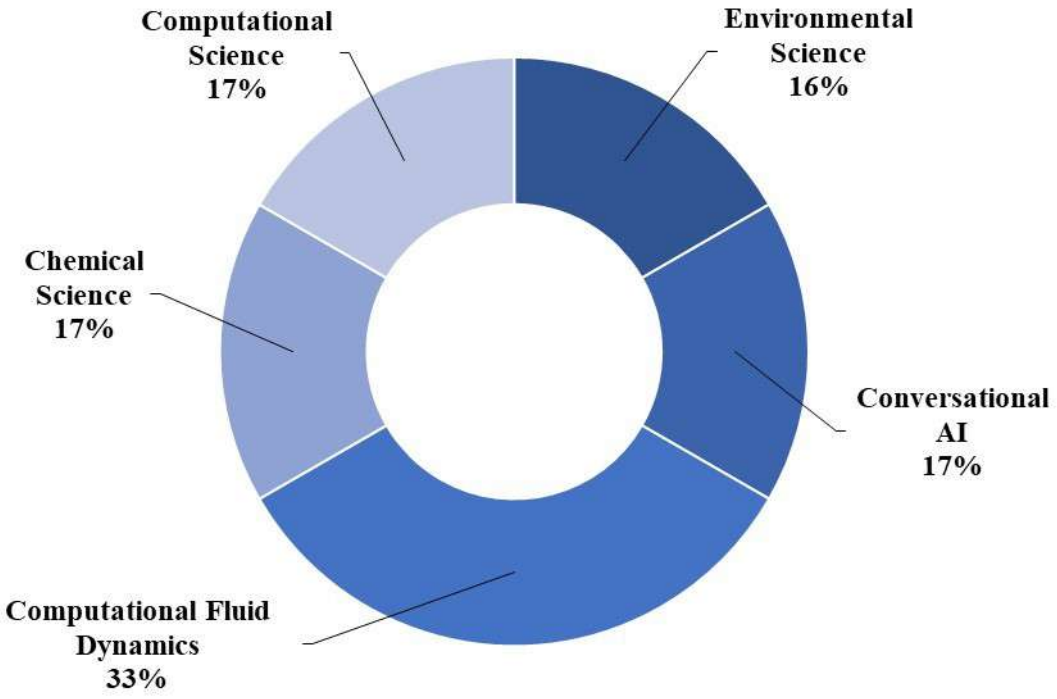


Figure: Number of publications across research fields

Table: Number of publications across research fields

Application Research Fields	Publication Count 2021
Computational Fluid Dynamics	2
Conversational AI	1
Environmental Science	1
Chemical Science	1
Computational Science	1

Number of PhDs across research fields

One PhD was awarded to Pruthwik Mishra from IIIT, Hyderabad under the supervision of Prof Dipti Misra Sharma. His research work includes Infrastructure for IIITH MT systems" and running Bahu-bhashak (NLTM) in the research area of conversational AI.

PARAM SIddhi-AI as convergence of HPC & AI

PARAM Siddhi-AI is incorporated with Graphics Processing Units (GPUs) to boost the processing power. These are purpose-built processors that can run deep learning models, central to most AI applications, an order of magnitude faster than traditional CPUs, to cater the HPC and AI applications on HPC cluster . Below Venn diagram shows the various HPC applications that use AI models and run their applications on the PARAM Siddhi-AI system. A total of 13 HPC applications use AI models.

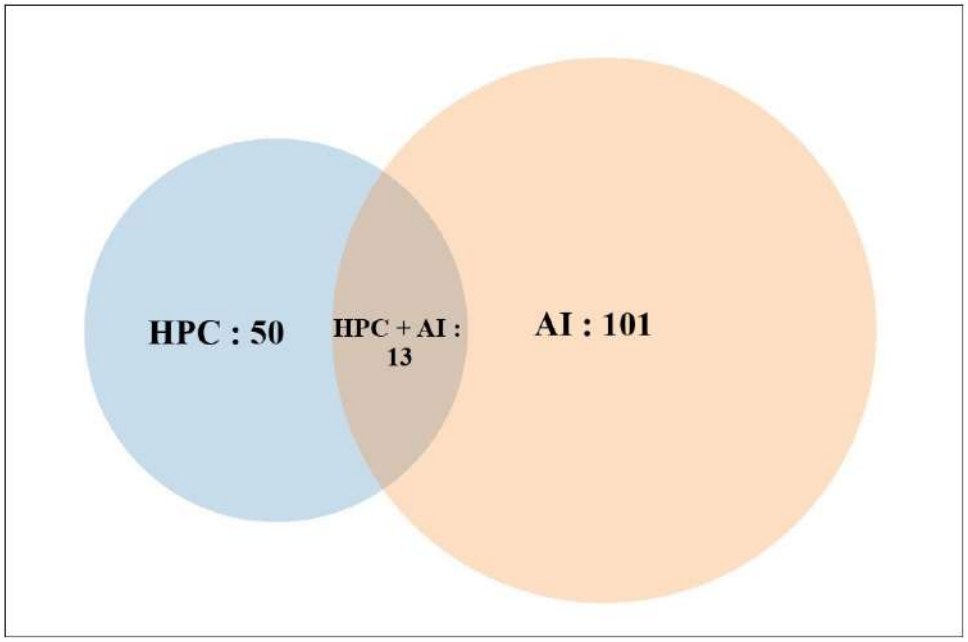


Figure: PARAM Siddhi-AI Convergence of HPC & AI

In the below Venn diagram, 3 applications of Computational Fluid Dynamics(CFD) , 3 applications of Environmental Sciences(ES), and 7 applications of BioInformatics(BI) are using AI models for their HPC applications, which have successfully run on PARAM Siddhi-AI system.

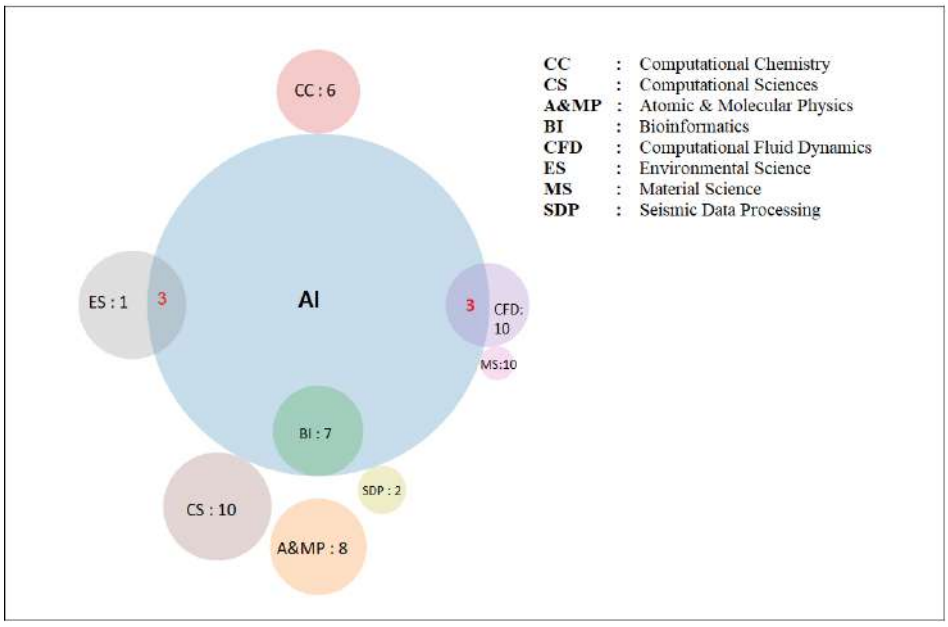


Figure: Distribution of HPC applications using AI models on PARAM Siddhi-AI

4

Science Using PARAM Siddhi-AI

4.1 Work Report Summary

Summary of PARAM Siddhi-AI work report is listed in this section, whearas, Details of work report are placed in **Annexure'A'**. Please click on details link to navigate on respective work report detail.

1. "Bahubhashak Pilot: Development and Deployment of English-Marathi-English Machine Translation System along with Creation of Robust Evaluation System" by Prof. Pushpak Bhattacharyya, Professor, pb@cse.iitb.ac.in , IIT Bombay Detail
2. "A Novel Scalable High-Performance Machine Learning Algorithms for NGS Analysis of Genomics Data at Exascale Level", by Dr. Aruna Tiwari, Professor, artiwari@iiti.ac.in , Indian Institute of Technology Indore Detail
3. "The numerical investigation of natural convection phenomena in the simple/complex porous media using deep learning techniques", by Dr. S.V.S.S.N.V.G. Krishna Murthy, skmurthy@diat.ac.in, Defence Institute of Advanced Technology Detail
4. "Design and Development of Quantum Computing Toolkit (simulator and workbench) and capacity building" by Mrs. Lakshmi Eswari P R, Director", prleswari@cdac.in, C-DAC Hyderabad Detail
5. "Early warning system for flood prediction in river basins of India" by Ms. Upasana Dutta, upasanad@cdac.in , C-DAC Pune Detail
6. "A high-performance, scalable FFT library & Pseudo-spectral code (Tarang) for modern GPUs" by Mahendra K. Verma, Professor, mkv@iitk.ac.in, IIT Kanpur Detail
7. "qttransport", by Dr. Jawar Singh, Prof. and Dean R&D, jawar@ iitp.ac.in, Indian Institute of Technology Patna Detail
8. "Monocular depth estimation using multi scale transformer", Ashutosh Agarwal, Student, csy202452@iitd.ac.in , IIT Delhi Detail
9. "PSA Bahubhashak Pilot", by Dipti Misra Sharma, Professor, dipti@iiit.ac.in, IIIT-Hyderabad Detail
10. "Adapt2Adverse: Improving Domain Generalization in Urban-Scene Segmentation in Adverse Weather Conditions", by Dr. Chetan Arora, Associate Professor, chetan@cse.iitd.ac.in, IIT-Delhi Detail
11. "Deep Learning Algorithms like Convolutional Neural Networks", by Dr. Manjari Gupta, Associate Professor, manjari@bhu.ac.in, DST-CIMS, BHU Detail

12. “Emotion recognition and Classification of Humans, Using EEG signals from the Dataset: GAMEEMO”, by Dr. Manjari Gupta, Associate Professor, manjari@bhu.ac.in, DST-CIMS, BHU Detail

13. “Automatic Speech Recognition in Indian English, Tamil, Hindi, and Text to Speech Synthesis for conversational speech in Indian languages, in particular Hindi, Tamil, and Indian English”, by Hema A Murthy, Professor, hema@cse.iitm.ac.in, IIT Madras Detail

14. “IndicASR -Automatic Speech Recognition Models for Indian Languages”, by Mitesh M. Khapra, Associate Professor, miteshk@cse.iitm.ac.in, Indian Institute of Technology, Madras Detail

15. “Hours to Milliseconds:Leveraging machine learning methods to reduce the computation time for crop yield prediction”, by Prof. Ganti S. Murthy, Professor, Ganti.murthy@iiti.ac.in, Indian Institute of Technology Indore Detail

16. “Sign Language Accessibility for e-Governance Services”, by Balan C, cbalan@cdac.in , CDAC Detail

17. “Bahubhashak(NMT)”, by Dr. Ajai Kumar, Senior Director, ajai@cdac.in, C-DAC, Pune Detail

18. “iOncology.ai”, by Dr. Ajai Kumar, Senior Director, ajai@cdac.in, C-DAC, Pune Detail

19. “Quantum Simulation and Computation of Atomic and Molecular Properties”, by Prof. Bhanu Pratap Das, Director, renu.bala@tcgcrest.org, Centre for Quantum Engineering, Research and Education (CQuERE), TCG CREST, Kolkata. Detail

20. “A HPC Software Suite for Seismic Imaging to Aid Oil & Gas Exploration”, by Richa Rastogi, richar@cdac.in, C-DAC , Pune Detail

21. “Advanced Materials and Probiotics through Machine Learning”, by Saroj Kumar Nayak, nayaks@itbbs.ac.in, Indian Institute of Technology Bhubaneswar (IIT-BBS) Detail

22. “High fidelity Simulations to capture transitional and turbulent flows in turbomachines”, by Dr. Nagabhushana Rao Vadlamani, Assistant Professor, nrv@iitm.ac.in, IIT Madras Detail

23. “HPC GPU Applications Benchmark Results on PARAM Siddhi”, by Manjunatha Valmiki, manjunathav@cdac.in, C-DAC, Pune Detail

24. “Design, development and deployment of end-to-end speech analytics suite” by Dr. Ajai Kumar, Senior Director, AAIG & GIST, C-DAC Pune, Ms. Lenali Singh, C-DAC Pune & Mr. Mahesh Bhargava, C-DAC Pune Detail

25. ”R&D on building DNN based speech recognition system under National Supercomputing Mission (NSM)” by by Dr. Ajai Kumar, Senior Director, AAIG & GIST, C-DAC Pune, Ms. Lenali Singh, C-DAC Pune & Mr. Mahesh Bhargava, C-DAC Pune Detail

26. “Development of HPC centric real-space numerical methodologies towards exa-scale architectures for large-scale ab-initio modeling of materials”, by Dr. Phani Sudheer Motamarri, Assistant Professor, phanim@iisc.ac.in , Indian Institute of Science, Bangalore Detail

4.2 PhD Theses

1. **Title of the thesis : A theoretical study of 2d boron monochalcogenide BX(X=S,Se,Te) for energy storage applications**
   Ph.D Scholar Name :Pruthwik Mishra
   Name of the Supervisor : Deepti Mishra Sharma
   Application Research Area : Conversational AI
   Name of the Institute : IIITH

4.3 Publications

List of publications Peer-Reviewd by NPSF PARAM Siddhi-AI users

Publications in National and International Journals and conferences

Publications 2021

1. Neural Machine Translation in Low-Resource Setting: a Case Study in English-Marathi Pair, Banerjee, A., Jain, A., Mhaskar, S., Deoghare, S., Sehgal, A. and Bhattacharyya, P., Proceedings of Machine Translation Summit XVIII, 2021.

2. On the efficacy of riblets toward drag reduction of transitional and turbulent boundary layers, S M Ananth, Massimiliano Nardini, Aditya Vaid, Nagabhushana Rao Vadlamani, Richard Sandberg", AIAA SciTech conference AIAA 2022-0472 , https://doi.org/10.2514/6.2022-0472

3. Dynamics of Bypass Transition with roughness and pulses of free-stream turbulence, Aditya Vaid, S. M. Ananth and Nagabhushana Rao Vadlamani", AIAA SciTech Forum 2022, 2021, https://arc.aiaa.org/doi/10.2514/6.2022-0453.

4. Performance Analysis of Python-based Finite Volume Solver ANUGA on Modern Architectures, Nisha Agrawal, Abhishek Das, Girishchandra R. Yendargaye, T. S. Murugesh Prabhu, Sandeep K. Joshi, and V. Venkatesh Shenoi. 2021. In 2021 Thirteenth International Conference on Contemporary Computing (IC3-2021) (IC3 '21). Association for Computing Machinery, New York, NY, USA, 378–387. DOI:https://doi.org/10.1145/3474124.3474152

5. Running a Single Instruction Execution Stream to a Massively Parallelized Computational Operations,Nisha Agrawal, Abhishek Das, Rishi Pathak, Manish Modani,(Conference Proceeding), 2021 IEEE Second International Conference on Technology, Engineering, Management for Societal Impact using Marketing, Entrepreneurship and Talent, at Symbiosis International (Deemed University), Pune, 10.1109/TEMSMET53515.2021.9768703

6. Molecular Dynamics Simulations Accelerate on Elastic Multi-GPU Architecture build with FP64/ TF32 latest Generation Streaming Multiprocessor Ampere Infrastructure , Nisha Agrawal, Abhishek Das, Rishi Pathak, Pankaj Dorlikar, Manish Modani, 6th International Conference on ICTCS 2021 & SMARTCOM 2021, Jaipur , India

5

Statistics of PARAM Yuva-II

5.1 System

System Availability

The pie chart is an indicator of system uptime (availability), one of the most important aspects of HPC facility. In 2020, NPSF PARAM Yuva II services were affected due to failure of the storage system and InfiniBand FDR Switch. These failures have impacted on the overall availability of the system and services to the user community. But, It can be seen that 2021 system availability is 100% without any failure of resources at NPSF, i.e. without any planned / unplanned downtime.

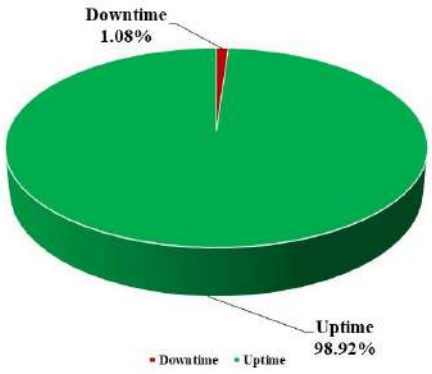


Figure: System Availability 2020

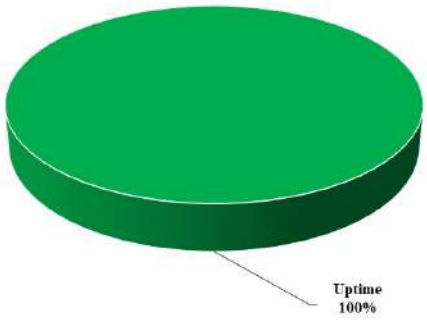


Figure: System Availability 2021

Table: System availability

Duration	Total Time	Downtime
1 Jan'20 - 31 Dec'20	366 Days (total : 8784 Hours)	3.92 Days (93 Hours)
1 Jan'21 - 31 Dec'21	365 Days (total : 8760 Hours)	0 Days (0.00 Hours)

System Utilization

System utilization (% CPU utilization) is calculated as % of CPU cores used by the batch jobs for computation, out of total available number of CPU cores, as indicated by the scheduler. This utilization is recorded every minute in the database. From the below GNU plot, It can be seen that the system utilization most of the times remained above 100% throughout the year. The gaps in the plot are indicative of the non-availability of the PARAM Yuva-II system , also sometimes non-availability of the data too.

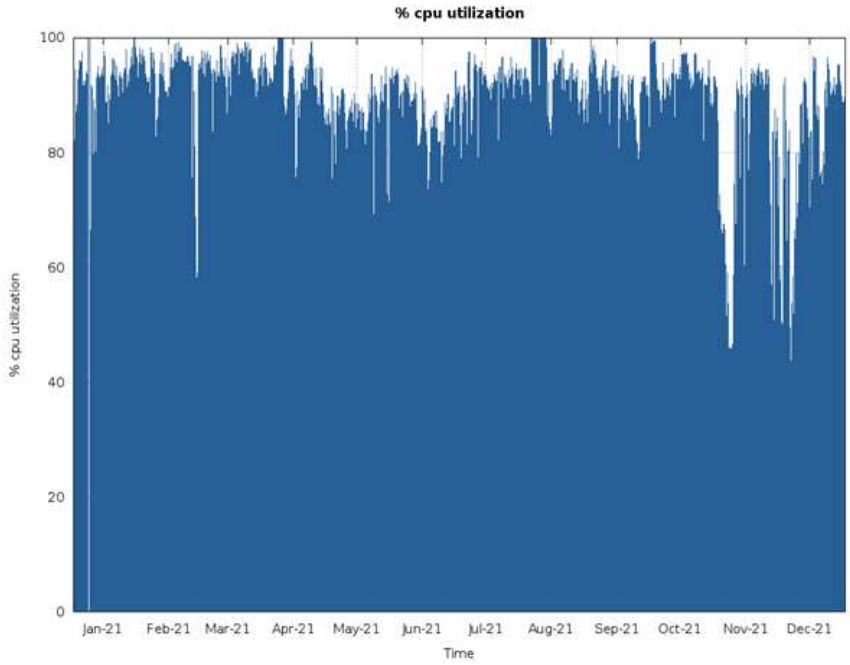


Figure: System Availability

CPU time utilization w.r.t. job sizes

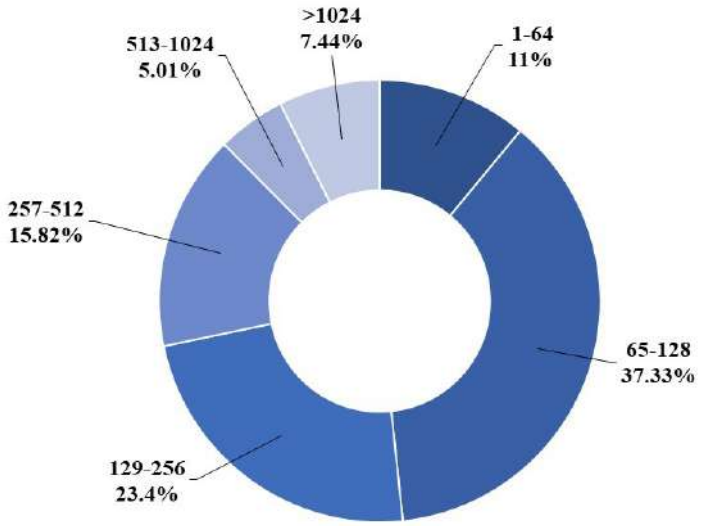


Figure: CPU Time Utilization w.r.t. Job Sizes (2020)

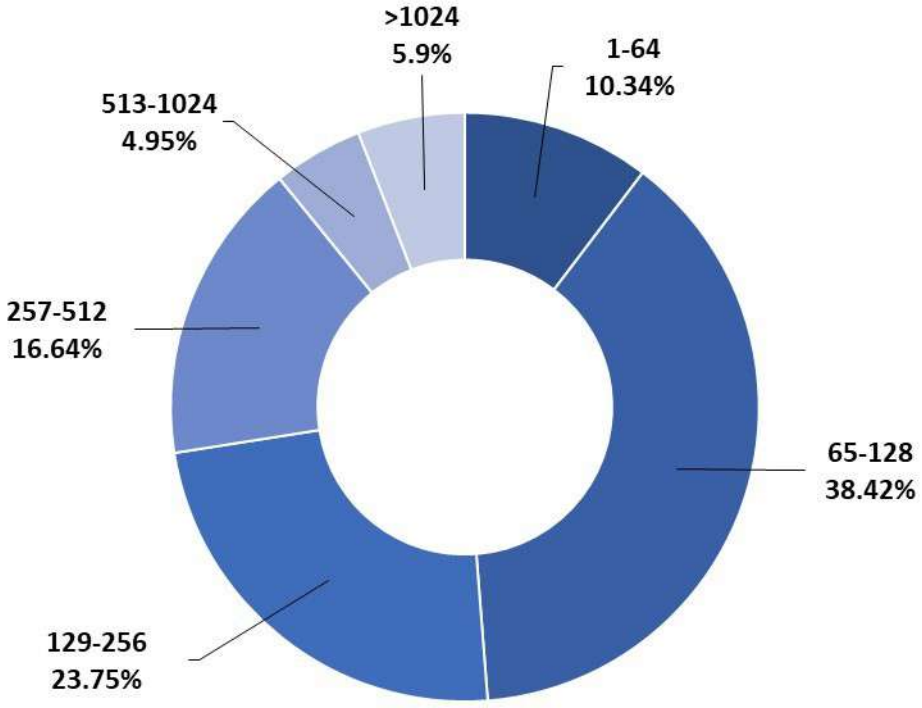


Figure: CPU Time Utilization w.r.t. Job Sizes (2021)

Table: CPU Time Utilization w.r.t. Job Sizes

	CPU time utilized (in CPU seconds)	
Job Sizes	**2020**	**2021**
1-64	16013713917	11100231303
65-128	54380930324	41240290093
129-256	34080972440	25484865174
257-512	23042286320	17855935936
513-1024	7299652256	5308182016
>1024	10836073472	6333273216

Above doughnut indicates % distribution of CPU time among different job sizes (binned by the number of cores). This graph also indicates an increase in % of computing capability.

% Distribution of jobs w.r.t. job sizes

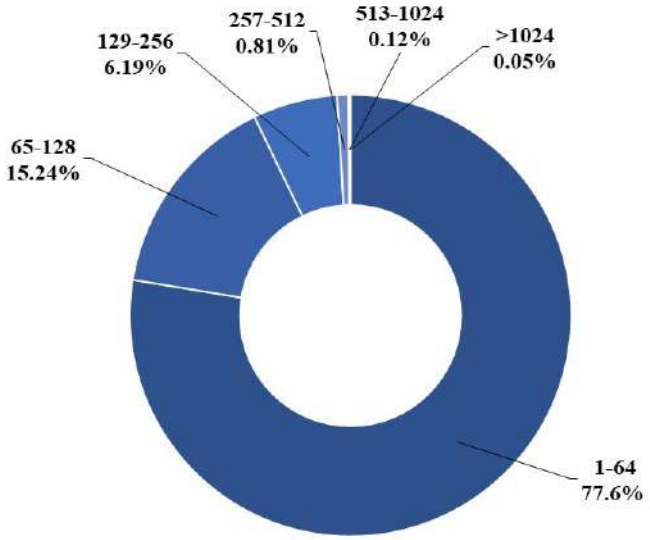


Figure: % Distribution of jobs w.r.t. job sizes (2020)

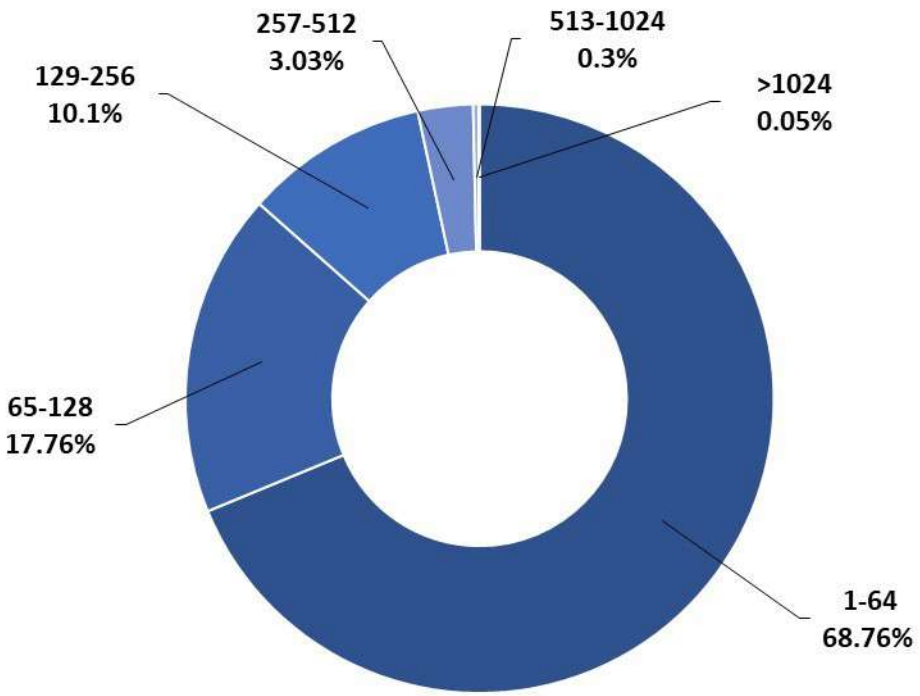


Figure: % Distribution of jobs w.r.t. job sizes (2021)

Table: Distribution of jobs w.r.t. job sizes (in seconds)

	Job Count	
Job Sizes	**2020**	**2021**
1-64	31590	13462
65-128	6209	3478
129-256	2525	1975
257-512	331	595
513-1024	50	57
>1024	23	10

Above doughnut indicates % distribution of the number of batch jobs binned by the number of cores. The percentage of the number of job sizes 257-512 (jobs requiring 257-512 range of CPU cores) has almost doubled from the last year.

Active jobs, idle jobs & system backlog

A job on NPSF HPC system is a construct comprising of a parallel program, resource requirements in terms of memory & CPU cores and indicative time for which these resources are required for successful completion. The two plots below present figures for :
1) Active jobs being processed
2) Idle jobs eligible for execution and waiting to be allocated the resources requested.

Active jobs

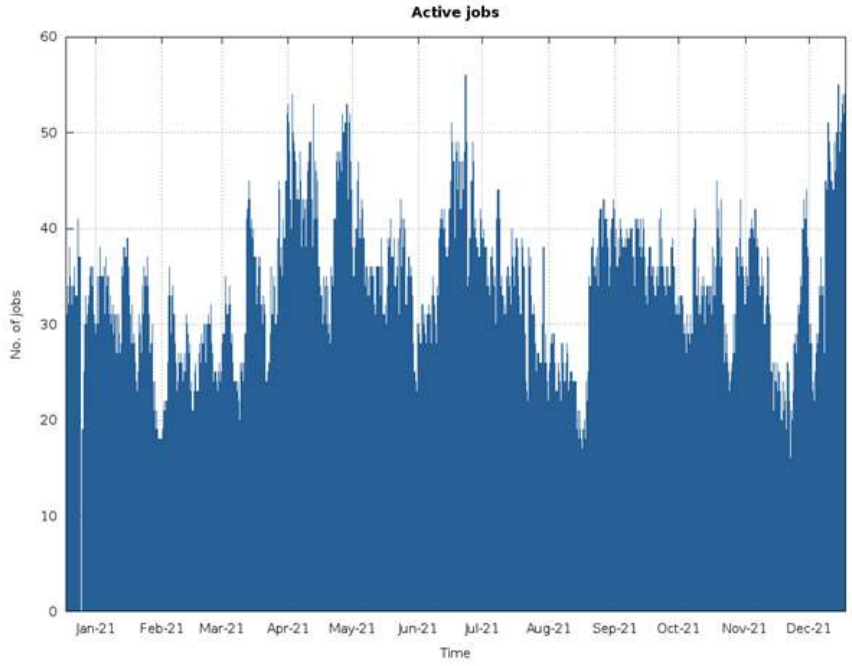


Figure: Active Jobs

Idle jobs

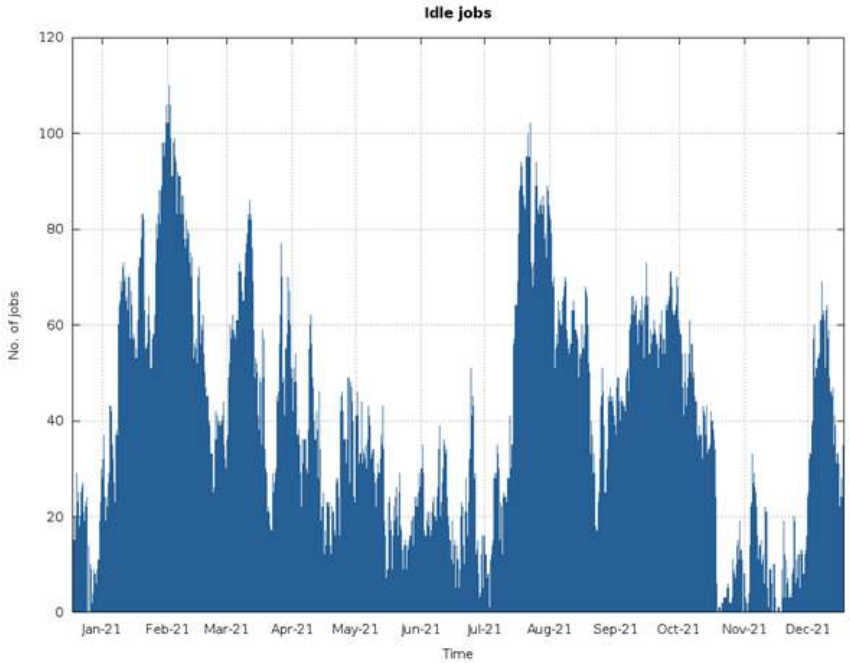


Figure: Idle Jobs

System backlog

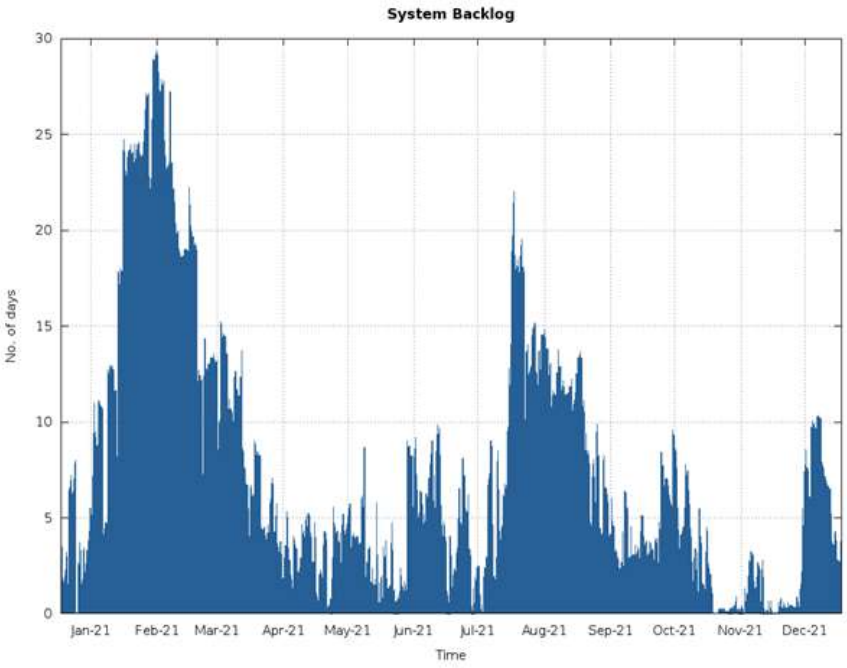


Figure: System Backlog

System backlog is computed as the total time required to process all idle jobs in the system, given that 1) No new jobs are introduced, & 2) State of the system is not changed, including compute capacity. The system backlog has reduced after the system unavailability due to decrease in number of jobs coming in, as there was no input and output data available after system was restored back to operation.

Absolute waittime Vs no. of jobs

Absolute wait time for a job is the time spent in the queue, after submission, till allocation of resources and execution. Above presentation is irrespective of job size. In 2021, as compared to last year, there is 80% decrease in the absolute wait time of the jobs that spend more than one day in the queue waiting for the resources. Also, in 2021, only 10% of the jobs have spent more than 1 day in queue.

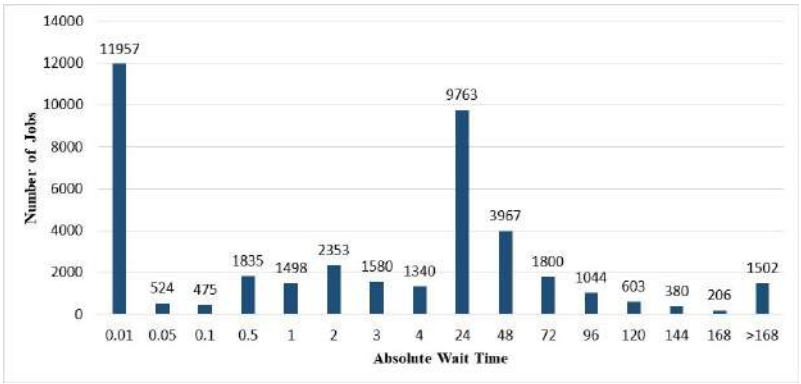


Figure: Absolute Wait Time(2020)

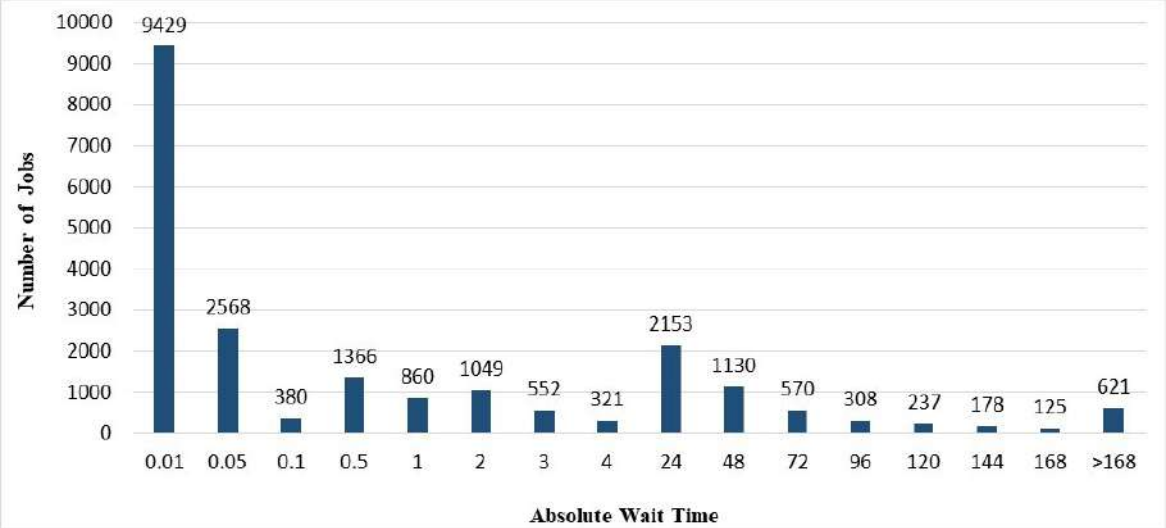


Figure: Absolute Wait Time(2021)

Table: Absolute waittime Vs no. of jobs

	No. of jobs	
Absolute wait time (in hours)	**Number of Jobs(2020)**	**Number of Jobs(2021)**
0.01	11957	9429
0.05	524	2568
0.1	475	380
0.5	1835	1366
1	1498	860
2	2353	1049
3	1580	552
4	1340	321
24	9763	2153
48	3967	1130
72	1800	570
96	1044	308
120	603	237
144	380	178
168	206	125
>168	1502	621

Execution Time Vs Number of Jobs

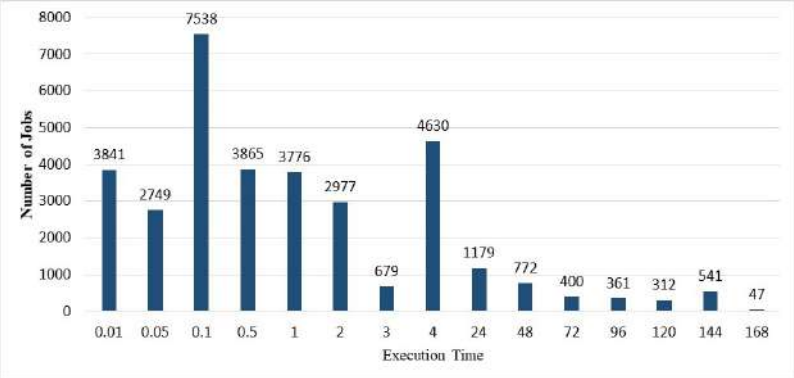


Figure: Execution Time V/s No. of Jobs(2020)

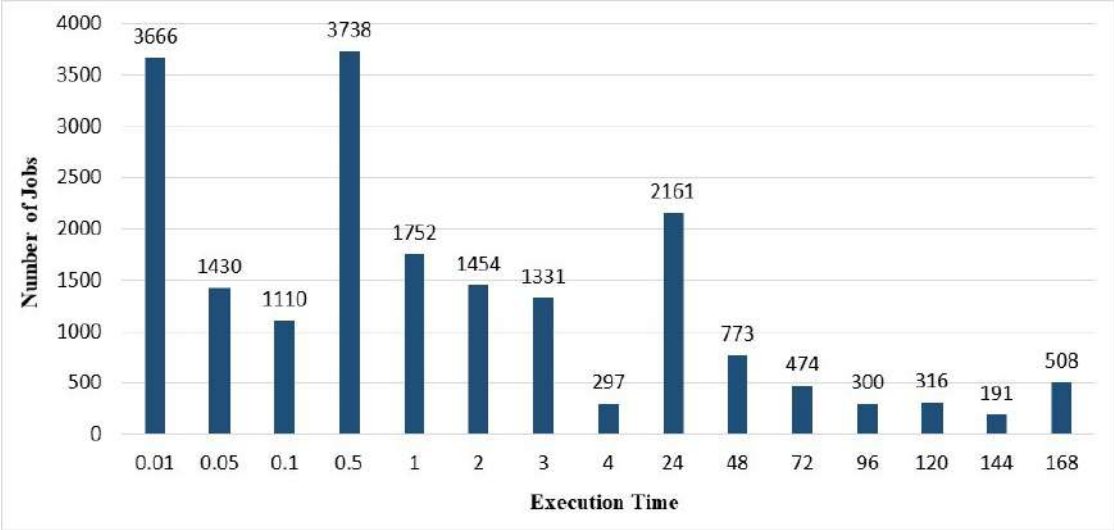


Figure: Execution Time V/s No. of Jobs(2021)

Table: Execution Time Vs Number of Jobs

	Number of Jobs	
Execution Time (in hours)	**Number of Jobs (2020)**	**Number of Jobs (2021)**
0.01	3841	3666
0.05	2749	1430
0.1	7538	1110
0.5	3865	3738
1	3776	1752
2	2977	1454
3	679	1331
4	4630	297
24	1179	2161
48	772	773
72	400	474
96	361	300
120	312	316
144	541	191
168	47	508

Above graph represents execution time of the jobs in hours.

Relative measure of job wait time with respect to it's execution time, binned by job sizes

Below representation is relative measure of job wait time with respect to its execution time, binned by job sizes. X-axis has the ratio of job waittime : execution time, Y-axis is the number of such jobs and on Z-axis, jobs are binned by number of CPU cores. It can be seen that majority of jobs spends time in waiting, which is >10 times their execution time. Bin sizes for above is 65 CPU cores onwards and statistics for jobs requesting less than that is given below.

This segregation is made because job count for 1 to 64 CPU cores, being very high, diminishes bars for other job sizes, thus making observable distance between them nondescript.

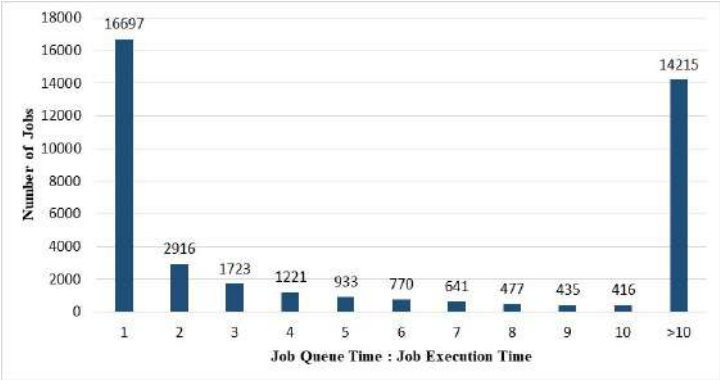


Figure: Relative measure of job wait time with respect to execution time, binned by job sizes(2020)

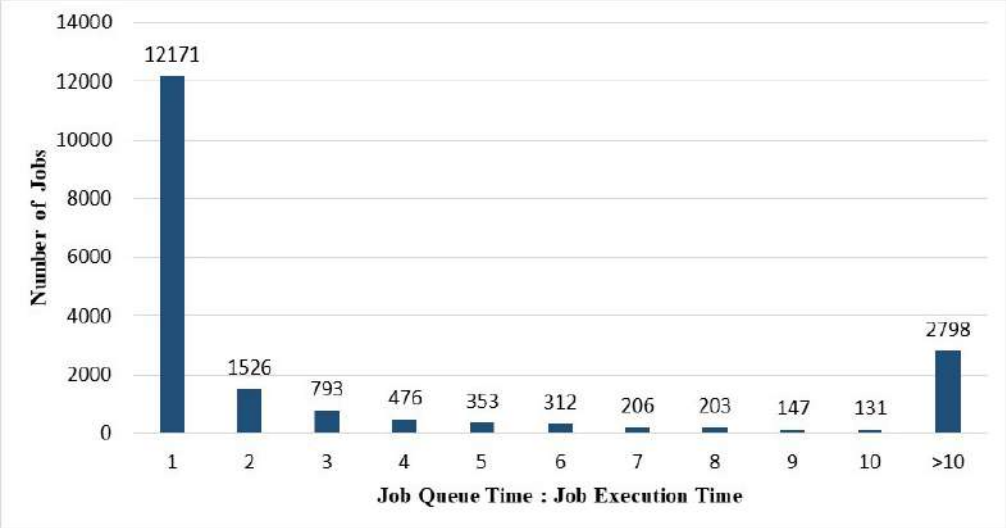


Figure: Relative measure of job wait time with respect to execution time, binned by job sizes(2021)

Table : Ratio of job waittime : execution time Vs number of jobs

2020	1	2	3	4	5	6	7	8	9	10	>10
1-64	11726	2067	1241	912	728	599	506	406	351	340	12306
65-128	3585	513	280	193	113	97	78	41	44	34	1147
129-256	1121	265	167	99	77	55	44	19	25	25	615
257-512	160	43	20	5	6	5	2	1	2	3	85
513-1024	45	11	6	3	0	4	2	0	1	1	23
>1024	7	2	0	1	2	0	0	1	1	1	8

Table : Ratio of job waittime : execution time Vs number of jobs

2021	1	2	3	4	5	6	7	8	9	10	>10
1-64	8764	1006	484	309	228	189	136	135	93	87	1587
65-128	2201	245	150	64	56	60	31	30	24	18	583
129-256	845	198	126	80	54	48	36	33	26	22	511
257-512	329	70	31	20	13	12	3	5	4	3	101
513-1024	30	5	1	3	1	3	0	0	0	1	12
>1024	2	2	1	0	1	0	0	0	0	0	4

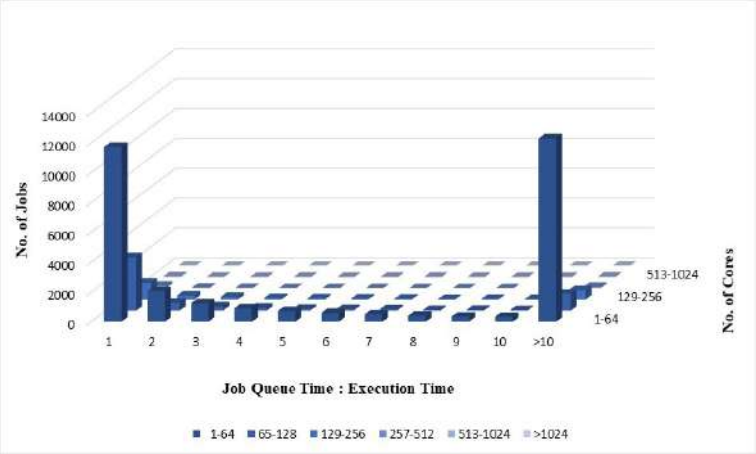


Figure: Ratio of job waittime : execution time Vs number of jobs(2020)

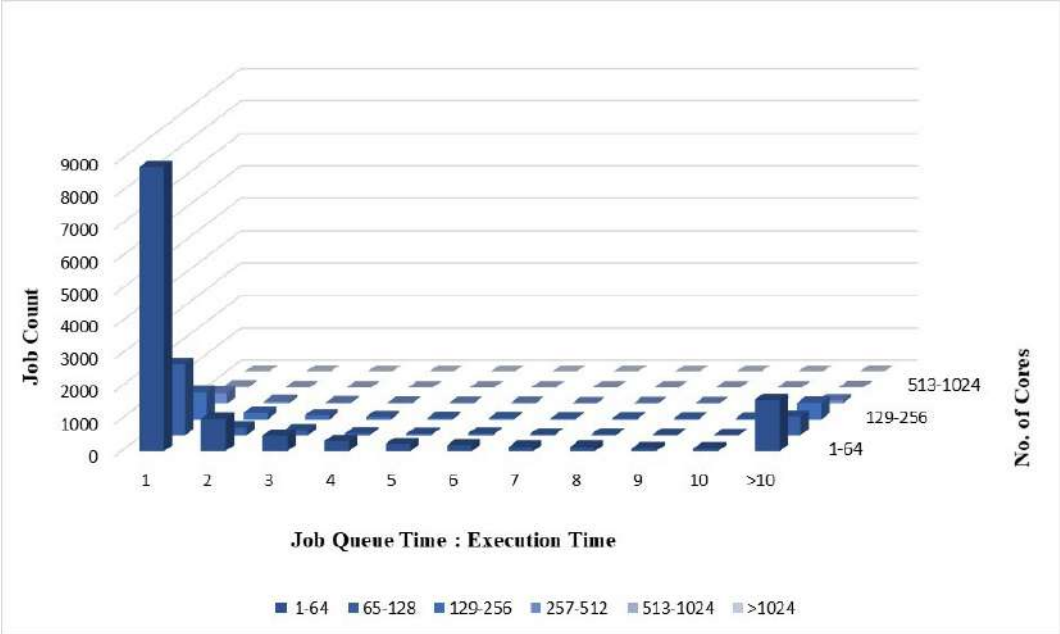


Figure: Ratio of job waittime : execution time Vs number of jobs(2021)

User support calls

Below Bar Graph shows the monthly wise distribution of support calls raised by users throughout the Year 2021. (NEED TO CHANGE THIS LINE)It can be seen that after Mar-2019 there was a sharp dip in the number of call raised it was due the unavailability of the system during that period.

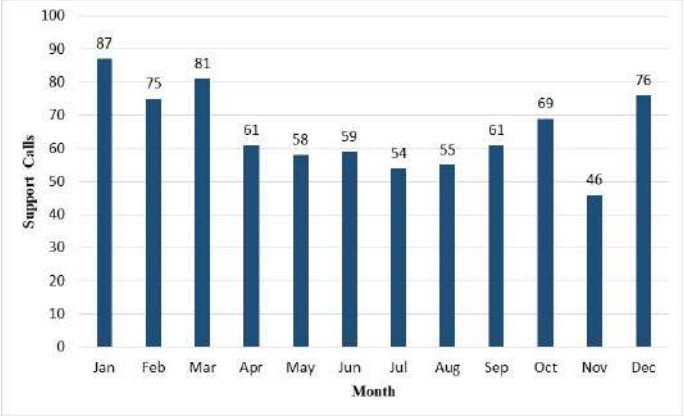


Figure: Month wise Support Calls (2020)

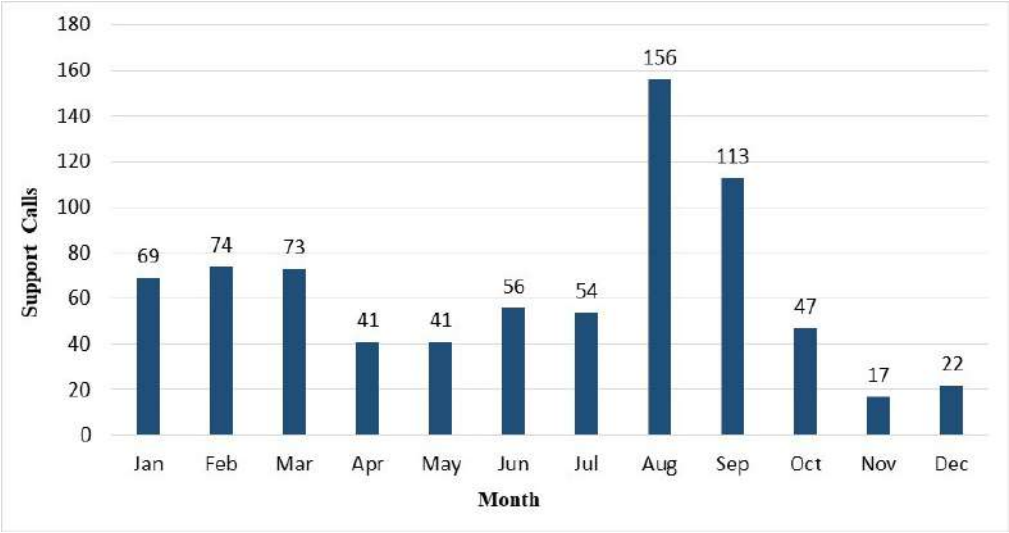


Figure: Month wise Support Calls (2021)

Table : Number of support calls

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
2020	87	75	81	61	58	59	54	55	61	69	46	76
2021	69	74	73	41	41	56	54	156	113	47	17	22

5.2 Users and Institutes

Institute wise CPU time utilization

User Jobs running over the cluster consumes CPU Time of the cluster. Below doughnut plot represents the % distribution of CPU Time consumed by the Research Organizations/Academic Institutes. As seen in the 2020 and 2021 plots, Jobs submitted from users of IIT Bombay is continuously consuming the max. % of CPU Time followed by Sri Guru Granth Sahib World University, Punjab .

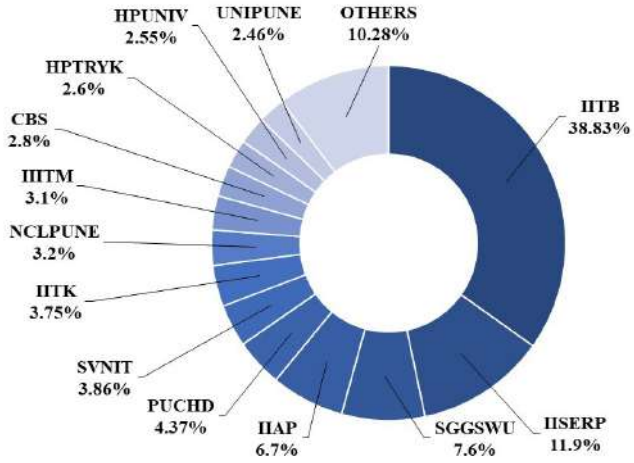


Figure: Institute wise CPU time utilization(2020)

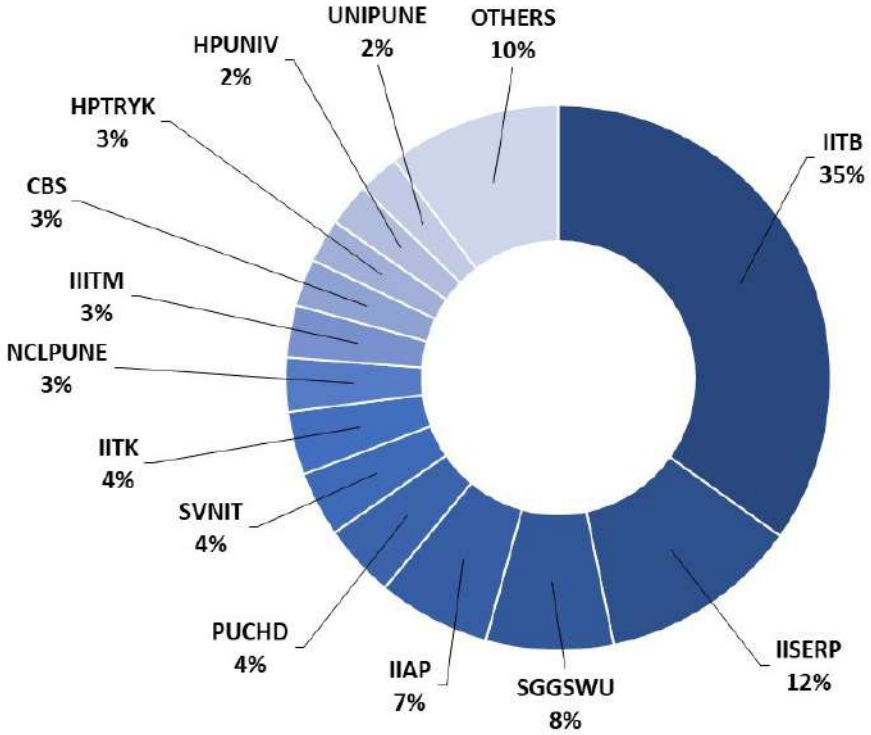


Figure: Institute wise CPU time utilization(2021)

Table : Institute vs. %CPU time utilization Year-2020

Institute	CPU Time Utilization(in CPU seconds)
IITB	42850701633
IISERP	14594041136
SGGSWU	9317473024
IIAP	8249226240
PUCHD	5383295120
SVNIT	4760117152
IITK	4622852034
NCLPUNE	3946017617
IIITM	3818456813
CBS	3446545744
HPTRYK	3193726574
HPUNIV	3146808947
UNIPUNE	3034532016
OTHERS	12647639197

Institute and job size wise job count

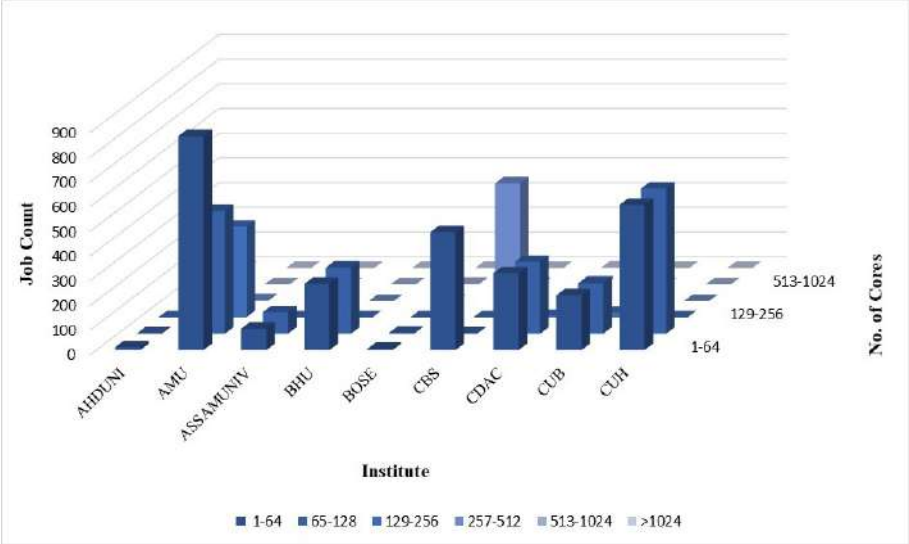


Figure: Institute and Job size wise Job count (2020)

Table : Institute wise %CPU time utilization Year-2021

Institute	CPU Time Utilization(in CPU seconds)
IITB	42850701633
IISERP	14594041136
SGGSWU	9317473024
IIAP	8249226240
PUCHD	5383295120
SVNIT	4760117152
IITK	4622852034
NCLPUNE	3946017617
IIITM	3818456813
CBS	3446545744
HPTRYK	3193726574
HPUNIV	3146808947
UNIPUNE	3034532016
OTHERS	12647639197

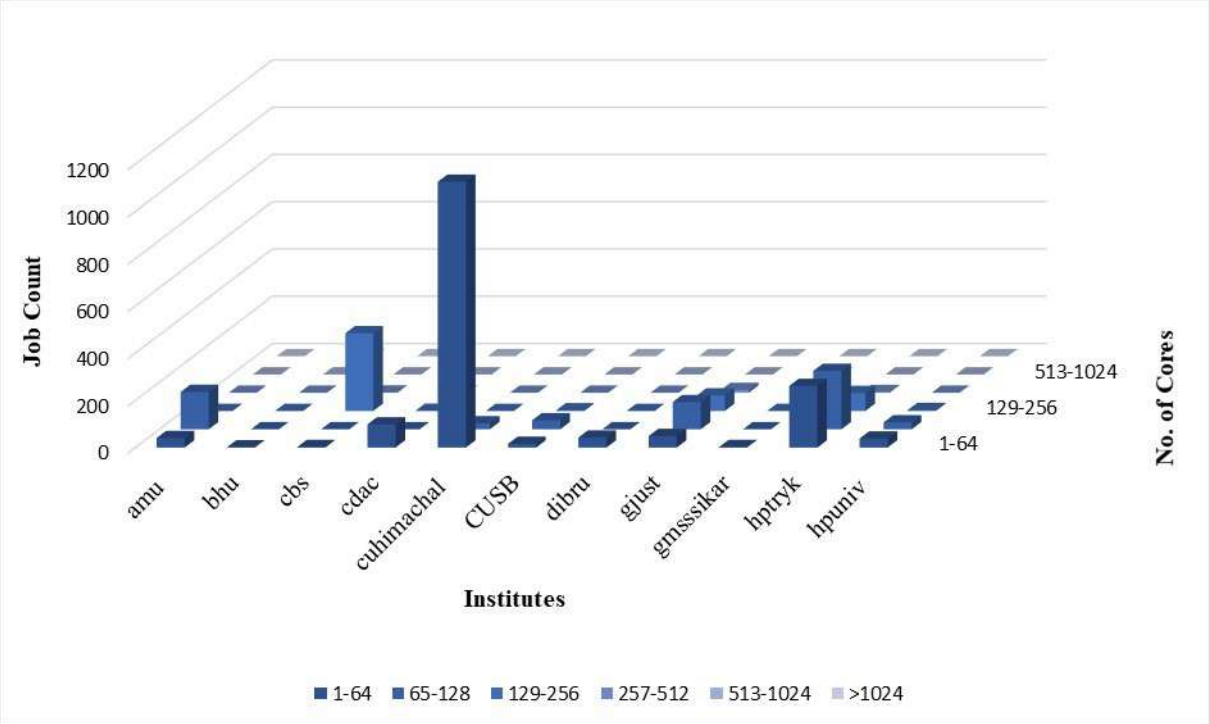


Figure: Institute and Job size wise Job count (2021)

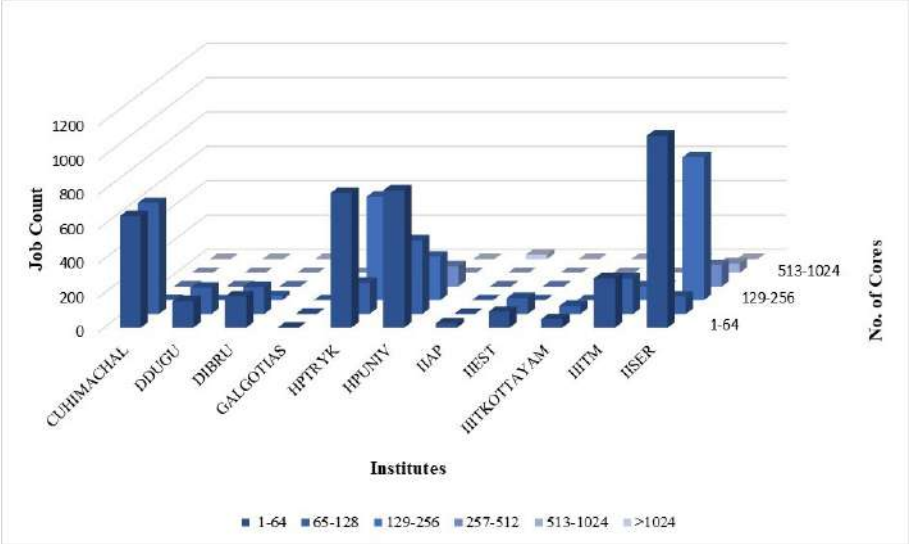


Figure: Institute and Job size wise Job count (2020)

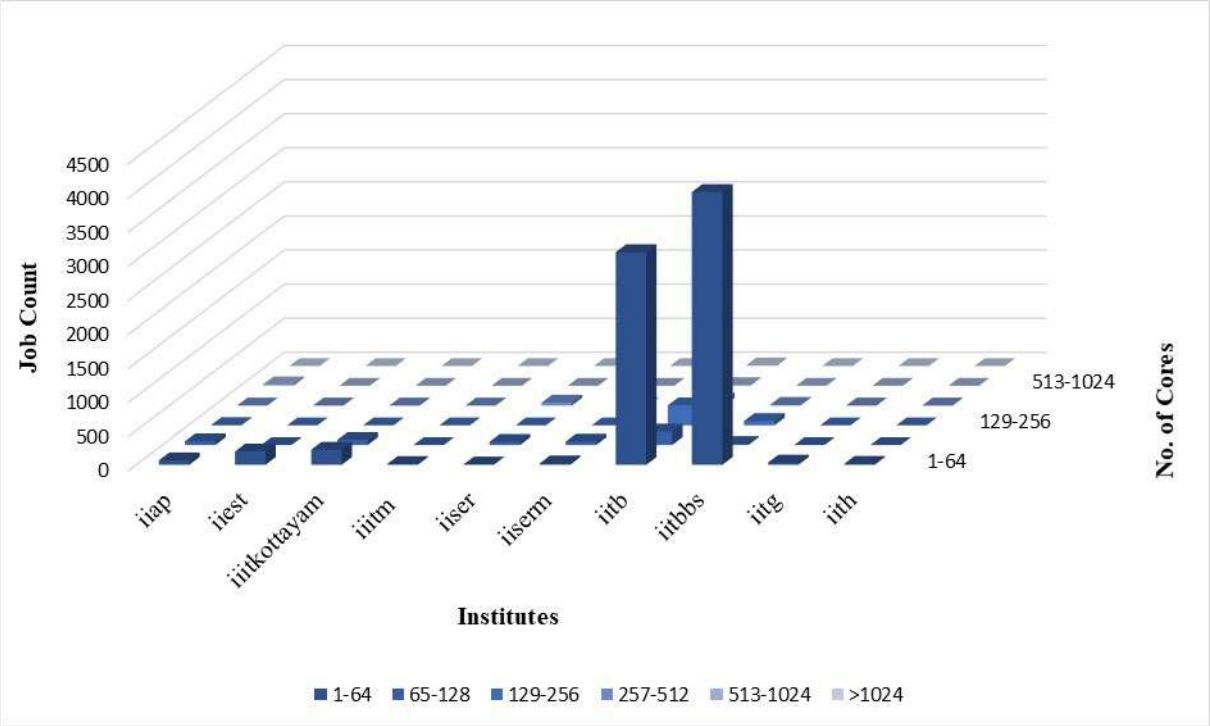


Figure: Institute and Job size wise Job count (2021)

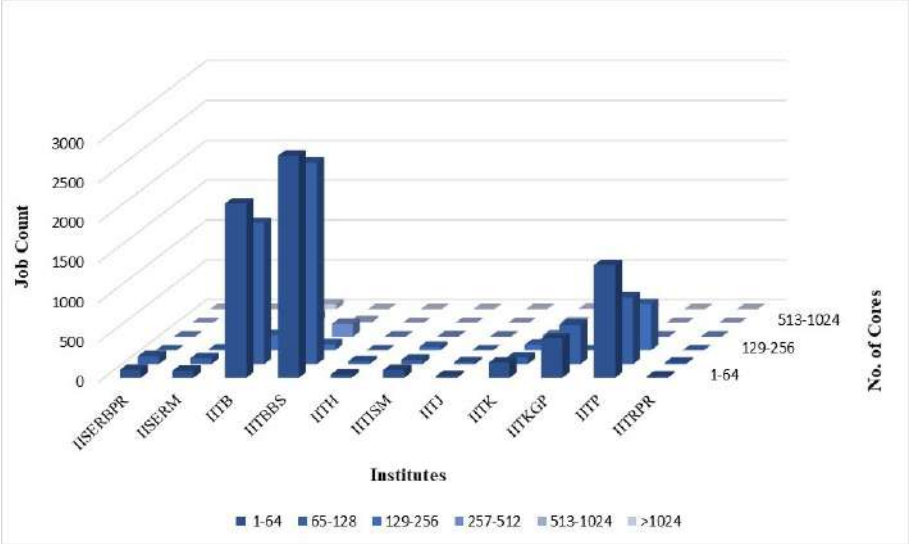


Figure: Institute and Job size wise Job count (2020)

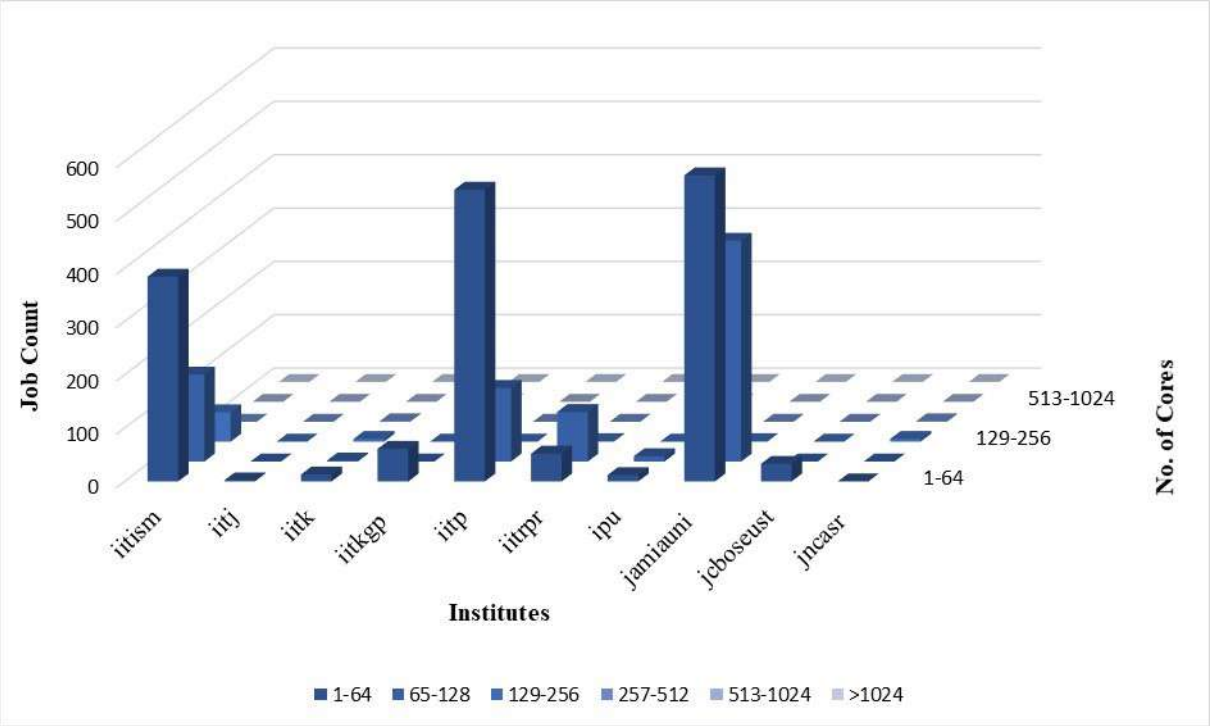


Figure: Institute and Job size wise Job count (2021)

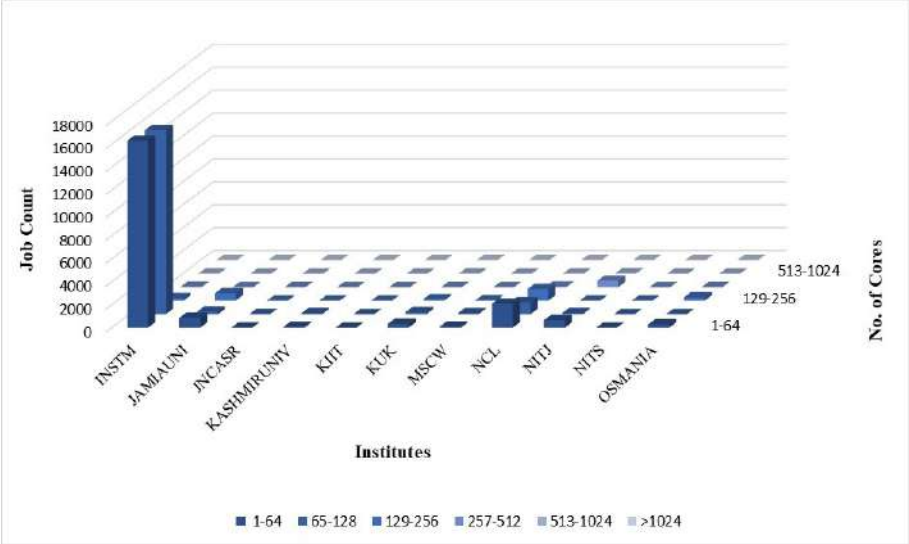


Figure: Institute and Job size wise Job count (2020)

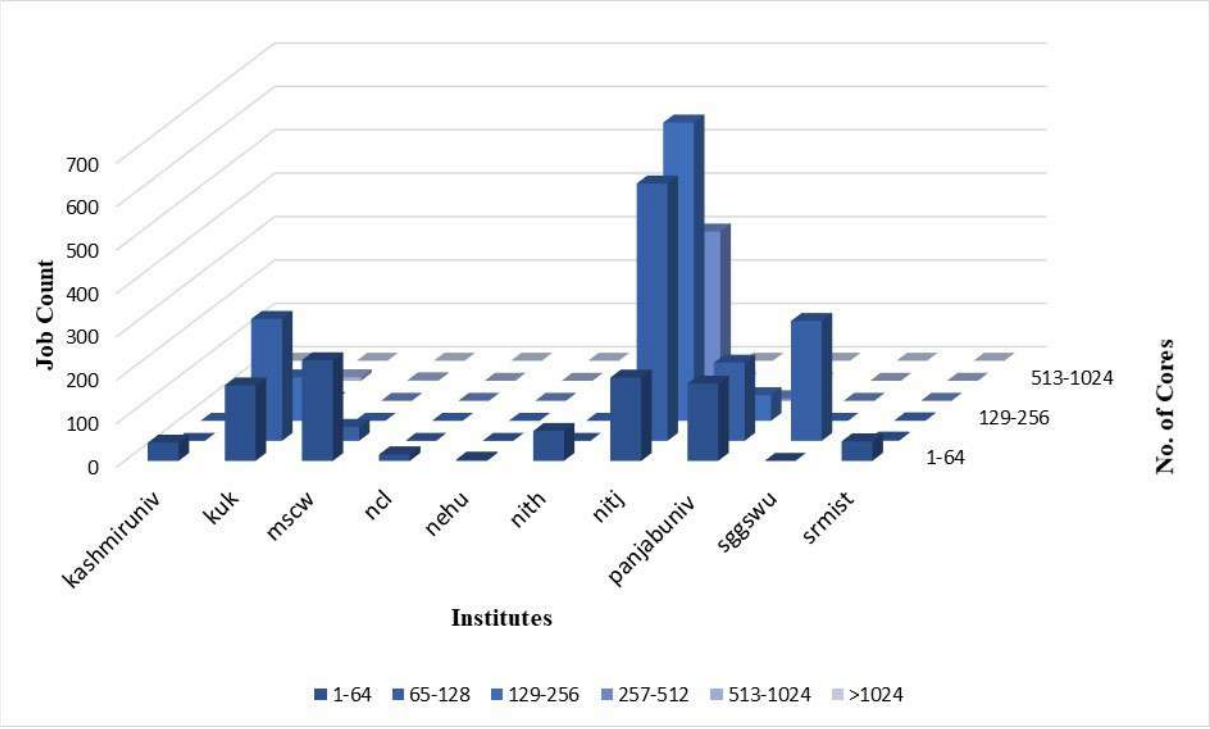


Figure: Institute and Job size wise Job count (2021)

Number of publications across institutes

User's Research work resulted to Publications, below doughnut plot represents the % wise publications across Research Organizations/Academic Institutes. In Year 2021 total 35 Publications have been published using PARAM Yuva II cluster in the reputed Journals and conferences.

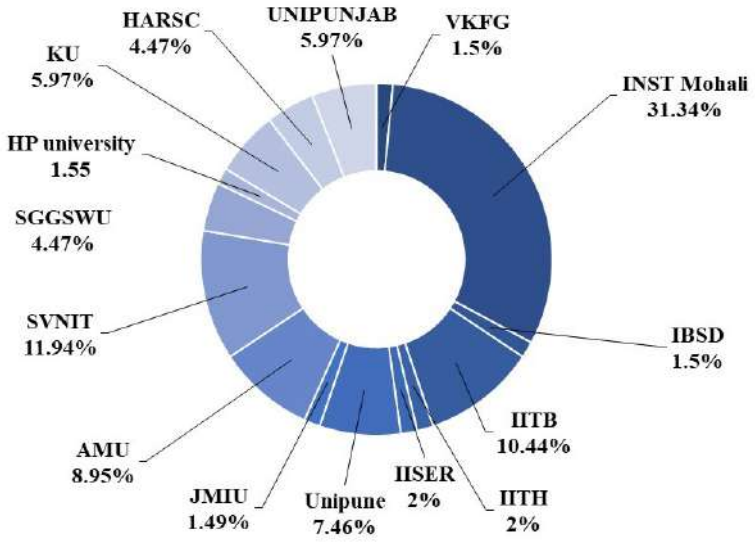


Figure: Number of publications accros Institutes (2020)

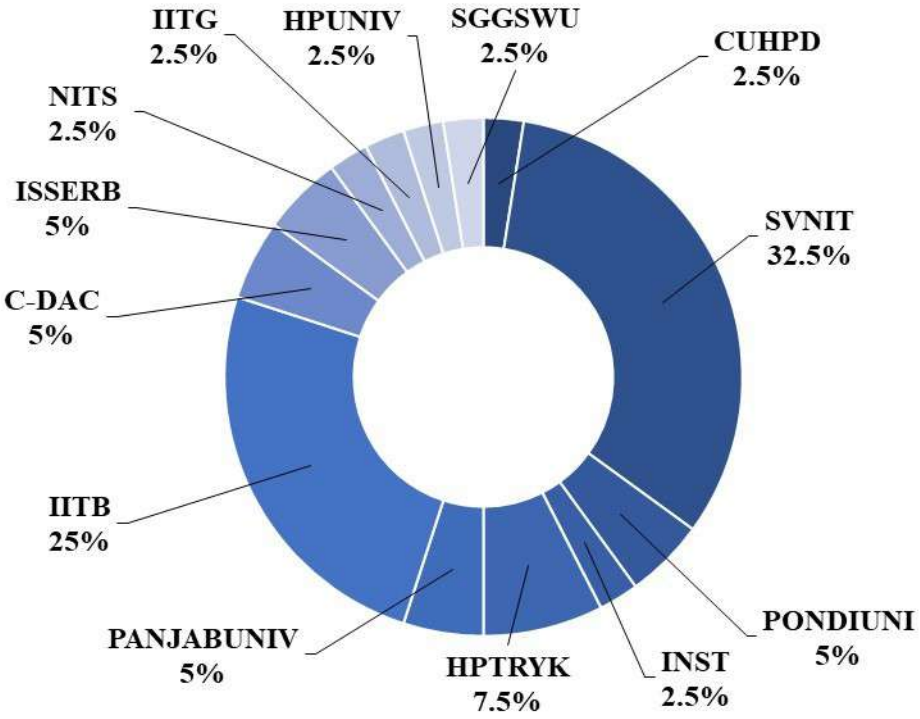


Figure: Number of Pubclications accros Institutes (2021)

Number of PhDs across institutes

In Year 2021, 6 of the PARAM Yuva II Users have completed Ph.D. and submitted the thesis, below are the details.

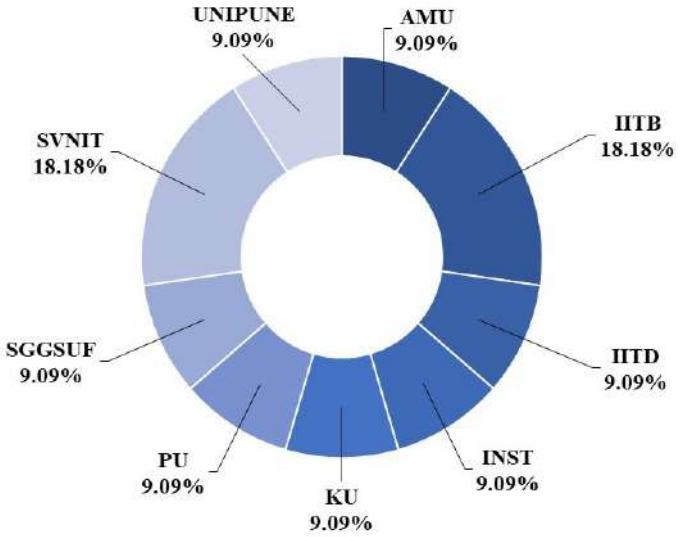


Figure: Number of PhDs across Institutes (2020)

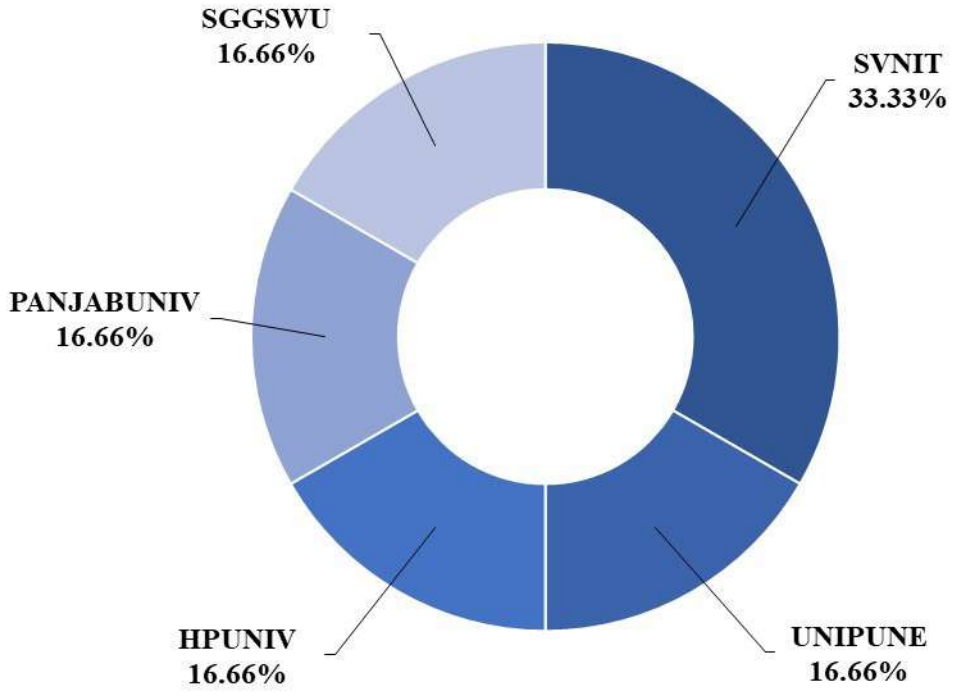


Figure: Number of PhDs across Institutes (2021)

5.3 Domain & Sectoral Usage

User's when affiliated with NPSF are classified according to their 1) Research Field, and 2) Institute. Former is deduced from area of work/application, whereas Institute is one of the attribute in Technical Affiliation Scheme (TAS) form. In this section, we have presented CPU time distribution, job count, and job size distribution across various Research Fields and Institutes. The inferences that can be derived from this data are to assess and corroborate percolation of HPC across application Research Fields and whether or not usage is perpetual during previous and current year.Job size distribution can be used to determine leaning towards capacity or capability computing requirements from HPC systems.

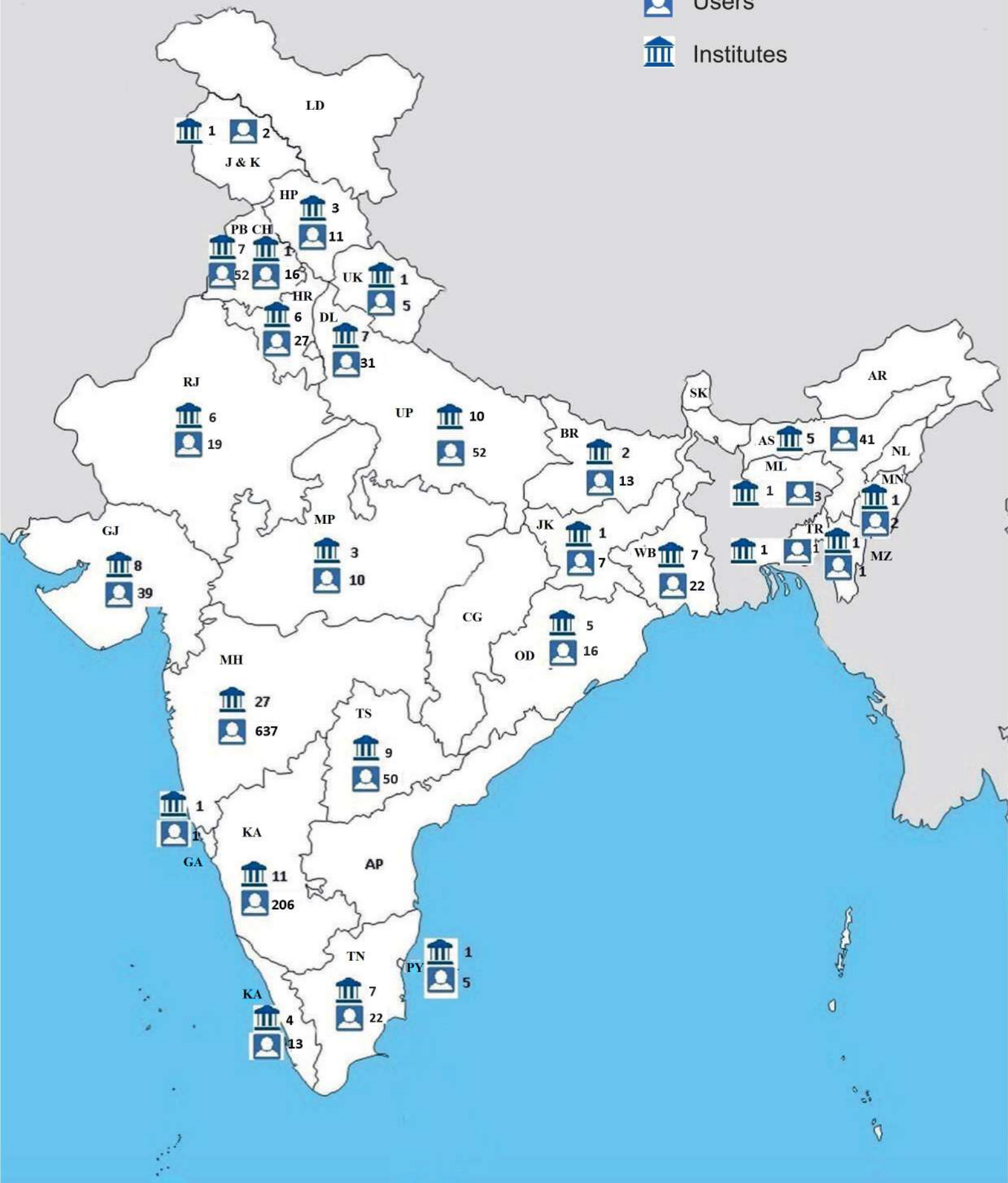
Table: List of application research fields on NPSF

S.No.	Research Fields
1	Astronomy & Astrophysics
2	Atomic & molecular Science
3	Bioinformatics
4	Computational Chemistry
5	Environmental Science
6	Complex System & Statistical Physics
7	Computational Fluid Dynamics
8	Computational Physics
9	Computational Science
10	Big Data Analytics
11	Geological Science
12	Material Science
13	Quantum Mechanics
14	Structural Engineering Mechanics
15	Computer Vision
16	Conversational AI
17	Uncategorized

Table: State wise Number of Users and Institutes

State	**Short Name**	**No .of Users**	**No.of Institutes**
Assam	AS	41	5
Bihar	BR	13	2
Chandigarh	CH	16	1
Delhi	DL	31	7
Goa	GA	1	1
Gujarat	GJ	39	8
Harayana	HR	27	6
Himachal Pradesh	HP	11	3
Jammu & Kashmir	J&K	2	1
Jharkhand	JK	7	1
Karnataka	KA	206	11
Kerala	KL	13	4
Maharashtra	MH	637	27
Manipur	MN	2	1
Meghalaya	ML	3	1
Mizoram	MZ	1	1
Madhya Pradesh	MP	10	3
Odisha	OD	16	5
Pondicherry	PY	5	1
Punjab	PB	52	7
Rajasthan	RJ	19	6
Tamil Nadu	TN	22	7
Telangana	TS	50	9
Tripura	TR	1	1
Uttar Pradesh	UP	52	10
Uttarakhand	UK	5	1
West Bengal	WB	22	7
	Total	1304	137

Users & Institutes



Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawnto scale nor conforms to international/ state borders in its entirety.

Table: State wise Number of Jobs Processed

State	**Short Name**	**No .of Jobs**
Assam	AS	75
Bihar	BR	742
Chandigarh	CH	423
Delhi	DL	1011
Gujarat	GJ	603
Haryana	HR	1016
Himachal Pradesh	HP	1290
Jammu and Kashmir	J&K	42
Jharkhand	JK	602
Karnataka	KA	417
Kerala	KL	297
Madhya Pradesh	MP	13
Maharashtra	MH	4058
Meghalaya	ML	3
Odisha	OD	4092
Punjab	PB	3460
Rajasthan	RJ	41
Tamil Nadu	TN	695
Telangana	TS	196
Tripura	TR	38
Uttar Pradesh	UP	220
West Bengal	WB	257

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Jobs Processed

Jobs Processed in %

Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawnto scale nor conforms to international/ state borders in its entirety.

Table: State wise Number of Active Projects

State	Short Name	No. of Projects
Assam	AS	3
Bihar	BR	3
Chandigarh	CH	6
Delhi	DL	3
Gujarat	GJ	2
Haryana	HR	4
Himachal Pradesh	HP	5
Jammu and Kashmir	J&K	1
Jharkhand	JK	2
Karnataka	KA	3
Kerala	KL	2
Madhya Pradesh	MP	1
Maharashtra	MH	24
Meghalaya	ML	1
Odisha	OD	2
Punjab	PB	5
Rajasthan	RJ	3
Tamil Nadu	TN	2
Telangana	TS	3
Tripura	TR	1
Uttar Pradesh	UP	3
West Bengal	WB	2

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Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawnto scale nor conforms to international/ state borders in its entirety.

Table: State wise Number of PhDs and Publications

State	**Short Name**	**No .of Publications**	**No .of PhDs**
Assam	AS	2	0
Gujrat	GJ	12	2
Himanchal Pradesh	HP	2	1
Maharsahtra	MH	15	1
Punjab	PB	4	2
Pondicherry	PY	2	0
Odisha	OD	2	0

Number of PhDs & Publications

Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawnto scale nor conforms to international/ state borders in its entirety.

Table: State wise CPU Time Utilisation

State	Short Name	CPU Time Utilisation(in CPU seconds)
Assam	AS	208875177
Bihar	BR	1804335752
Chandigarh	CH	5643620625
Delhi	DL	4022674407
Gujarat	GJ	4439368625
Haryana	HR	2015963791
Himachal Pradesh	HP	736398032
Jammu and Kashmir	J&K	149603808
Jharkhand	JK	4084356451
Karnataka	KA	3252170623
Kerala	KL	770448313
Madhya Pradesh	MP	32544
Maharashtra	MH	45993834945
Meghalaya	ML	19424
Odisha	OD	4960080129
Punjab	PB	23639415890
Rajasthan	RJ	161511961
Tamil Nadu	TN	122560034
Telangana	TS	147431784
Tripura	TR	2848
Uttar Pradesh	UP	5058098559
West Bengal	WB	124098992

CPU Time Utilization in %

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Research Field wise CPU time utilization

Below doughnut plot represents the % CPU Time utilization by the jobs across application research fields. In 2020, Chemical sciences and Material Science were the major contributors towards the CPU time utilization, whearas, in 2021 Computational Science and Chemical sciences are the mojor contributors towards the CPU time utilization.

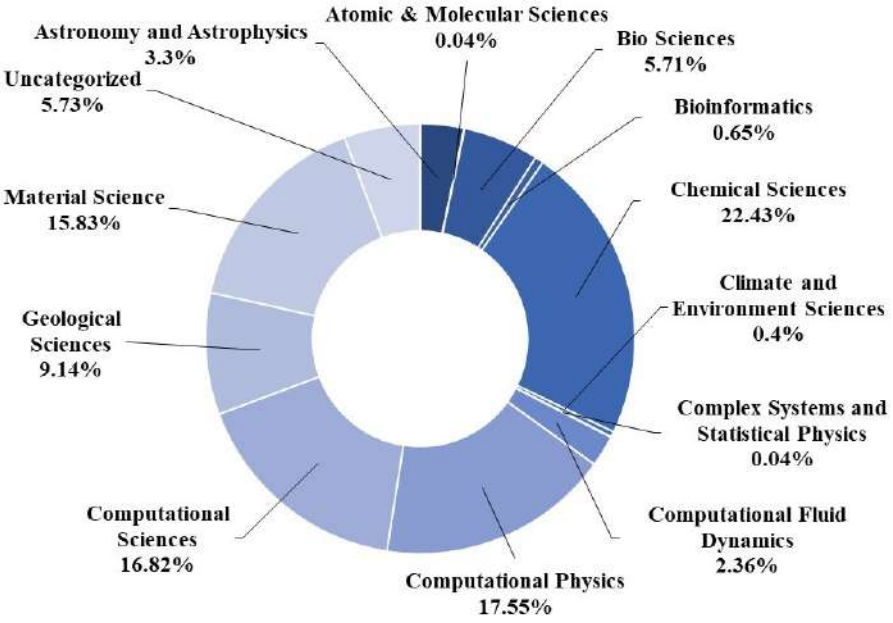


Figure: Research field wise CPU time utilization (2020)

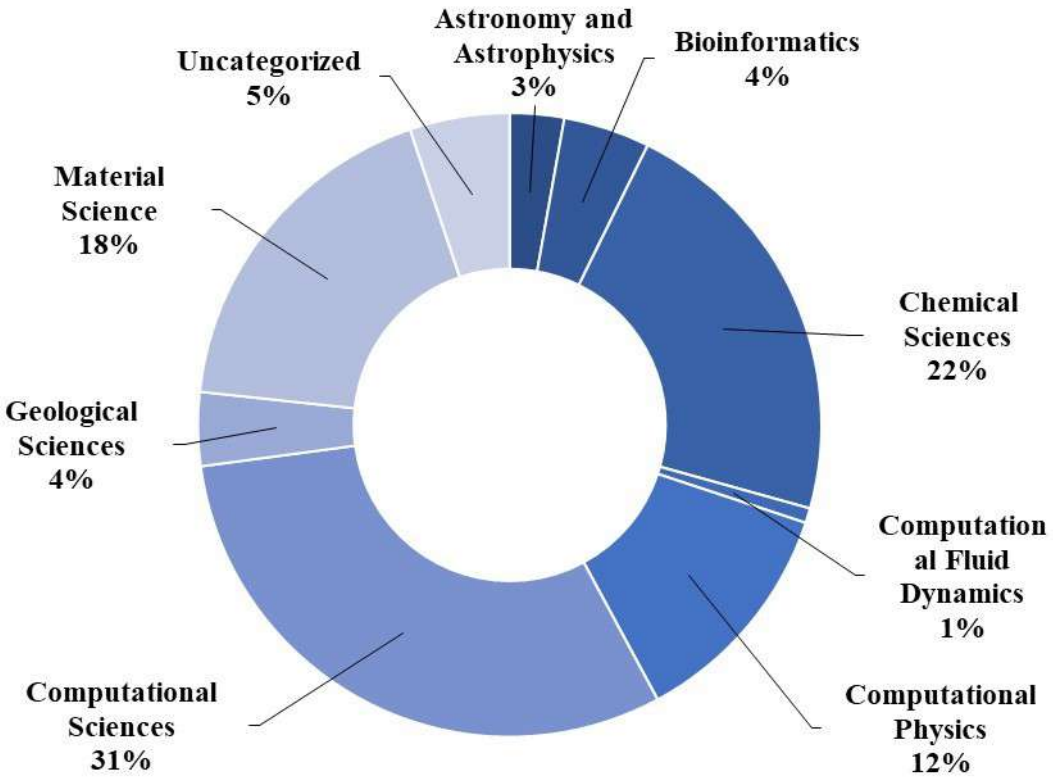


Figure: Research field wise CPU time utilization (2021)

Table: Research Field wise CPU time utilization

	CPU time in CPU seconds	
Application Research Field	**2020**	**2021**
Astronomy and Astrophysics	5552407552	3005049470
Atomic & Molecular Sciences	69546775	0
Bio Sciences	9654114436	0
Bioinformatics	1109614483	4802181752
Chemical Sciences	37888104207	23548019896
Climate and Environment Sciences	648796608	0
Complex Systems and Statistical Physics	67135296	0
Computational Fluid Dynamics	3994466286	822938956
Computational Physics	29639336426	12884025118
Computational Sciences	28398418242	32887418135
Geological Sciences	15426684008	4084356451
Material Science	26724497896	19385553324
Uncategorized	9682392056	5537992026

Job distribution across application research fields

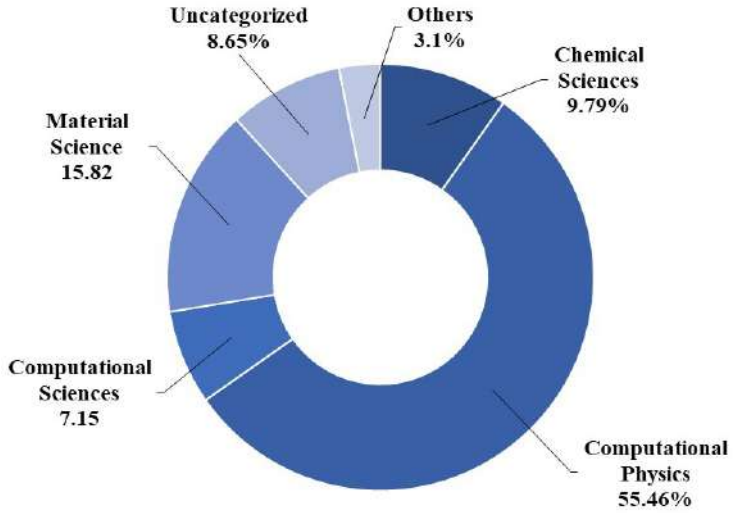


Figure: Job distribution across application research fields (2020)

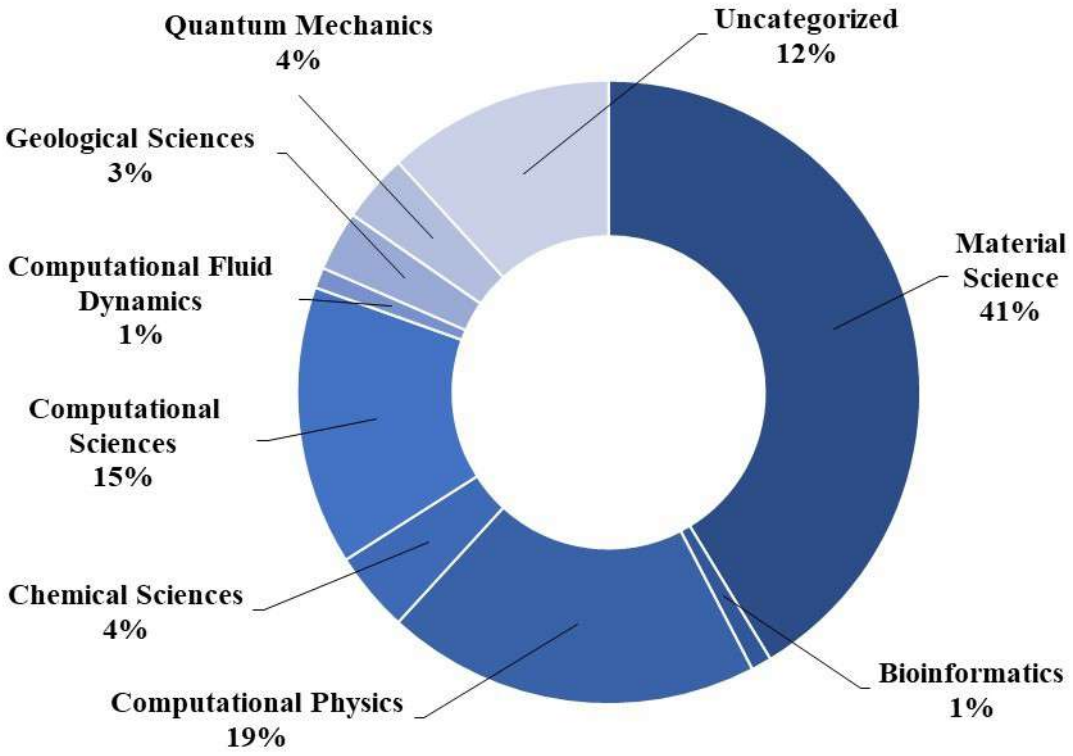


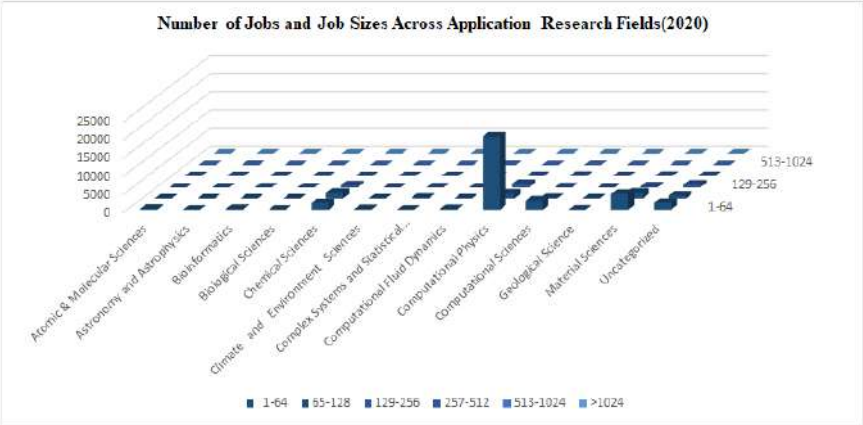
Figure: Job distribution across application research fields (2021)

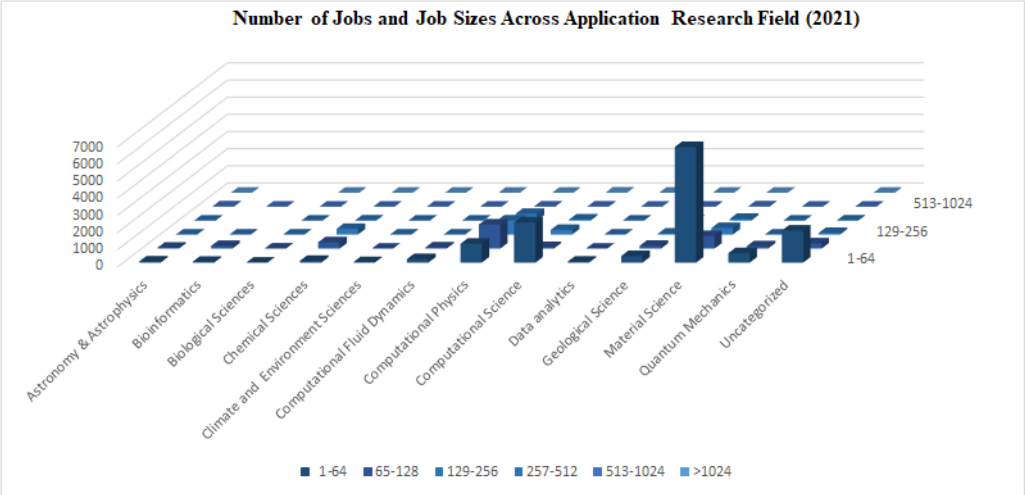
Above plots shows application research fields wise percentage distribution of number of jobs processed.

Table: Job distribution across application research fields

	No. of Jobs	
Application Research Field	**Job Count 2020**	**Job Count 2021**
Astronomy and Astrophysics	238	0
Atomic & Molecular Sciences	26	0
Bioinformatics	191	205
Biological Sciences	36	0
Chemical Sciences	3994	806
Climate and Environment Sciences	182	0
Computational Fluid Dynamics	232	206
Complex Systems and Statistical Physics	295	0
Computational Physics	22613	3748
Computational Sciences	2918	2794
Data analytics	0	0
Geological Sciences	68	602
Material Science	6451	7972
Quantum Mechanics	0	685
Uncategorized	3529	2277

Job sizes across application research fields





Above plots depicts distribution of jobs in reference to number of CPU cores requested, binned by ranges 1-64, 65-128, 129-256, 257-512, and 513-1024 & above.

Table: Number of Jobs and Job Sizes across Application Research Fields 2021

Application Research Fields	1-64	65-128	129-256	257-512	513-1024	>1024
Astronomy & Astrophysics	66	55	3	1	21	0
Bioinformatics	47	158	0	0	0	0
Biological Sciences	1	1	0	0	0	0
Chemical Sciences	96	372	330	8	0	0
Climate and Environment Sciences	24	0	1	0	0	0
Computational Fluid Dynamics	205	67	1	0	0	0
Computational Physics	1097	1404	827	398	8	0
Computational Science	2338	91	279	67	10	9
Data analytics	56	0	0	0	0	0
Geological Science	384	163	55	0	0	0
Material Science	6733	729	384	104	15	1
Quantum Mechanics	547	138	0	0	0	0
Uncategorized	1868	300	95	14	0	0

Table: Number of Jobs and Job Sizes across Application Research Fields (2020)

Application Research Fields	1-64	65-128	129-256	257-512	513-1024	>1024
Atomic & Molecular Sciences	238	0	0	0	0	0
Astronomy and Astrophysics	0	0	0	0	26	0
Bioinformatics	166	4	21	8	6	33
Biological Sciences	4	1	0	11	0	20
Chemical Sciences	1825	1644	521	4	0	0
Climate and Environment Sciences	157	25	0	0	0	0
Complex Systems & Statistical Physics	2	281	12	0	0	0
Computational Fluid Dynamics	160	42	0	2	28	0
Computational Physics	20180	1458	901	62	12	0
Computational Sciences	2529	198	51	101	37	2
Data analytics	0	0	0	0	0	0
Geological Science	22	43	2	1	0	0
Material Sciences	4408	1670	267	93	13	0
Uncategorized	1876	842	747	57	6	1

Number of publications across research fields

Below doughnut plot represents the % number of Publications across Application Research field. Since last two years, Majority of the Publications belongs to Computational Physics and Material Science domain.

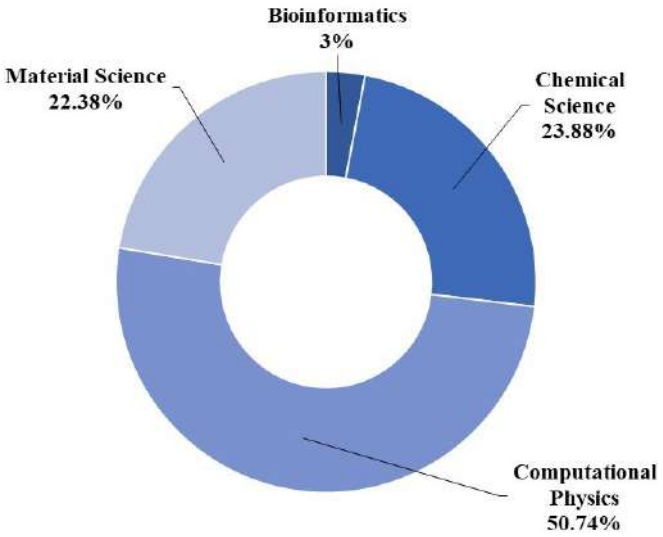


Figure: Number of Publications across research fields (2020)

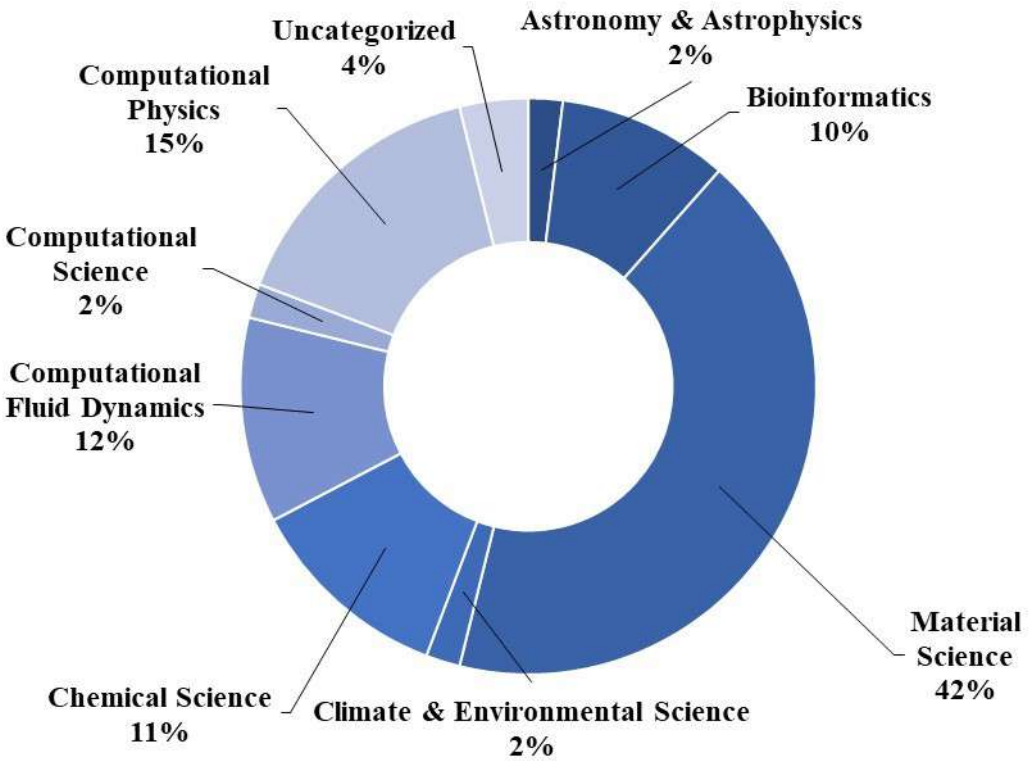


Figure: Number of Publications across research fields (2021)

Table: Number of publications across research fields

	Number of publicatons	
Application Research Fields	**Publication Count 2020**	**Publication Count 2021**
Astronomy & Astrophysics	0	1
Atomic and Molecular Science	0	0
Bioinformatics	2	5
Bio Science	0	0
Chemical Science	16	6
Climate & Environmental Science	0	1
Complex Systems & Statstical Physics	0	0
Computational Fluid Dynamics	0	6
Computational Physics	34	8
Computational Science	0	1
Geological Science	0	0
Material Science	15	22
Uncategorized	0	2

Number of PhDs across application research fields

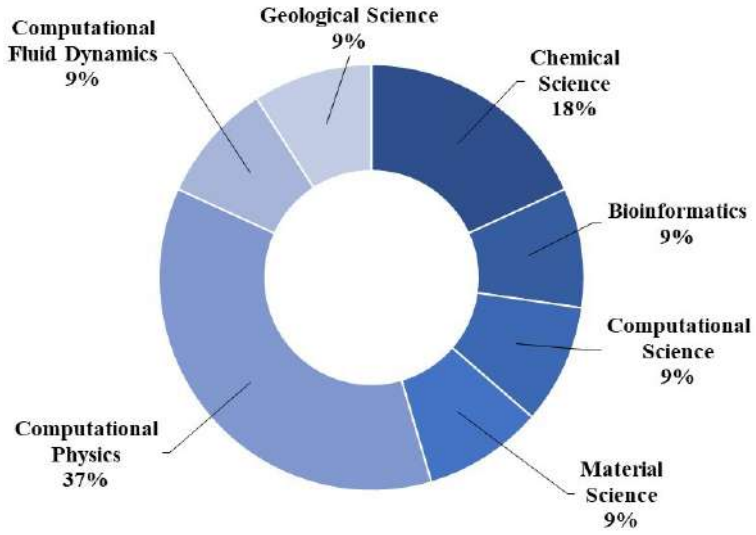


Figure: Number of PhDs across application research fields (2020)

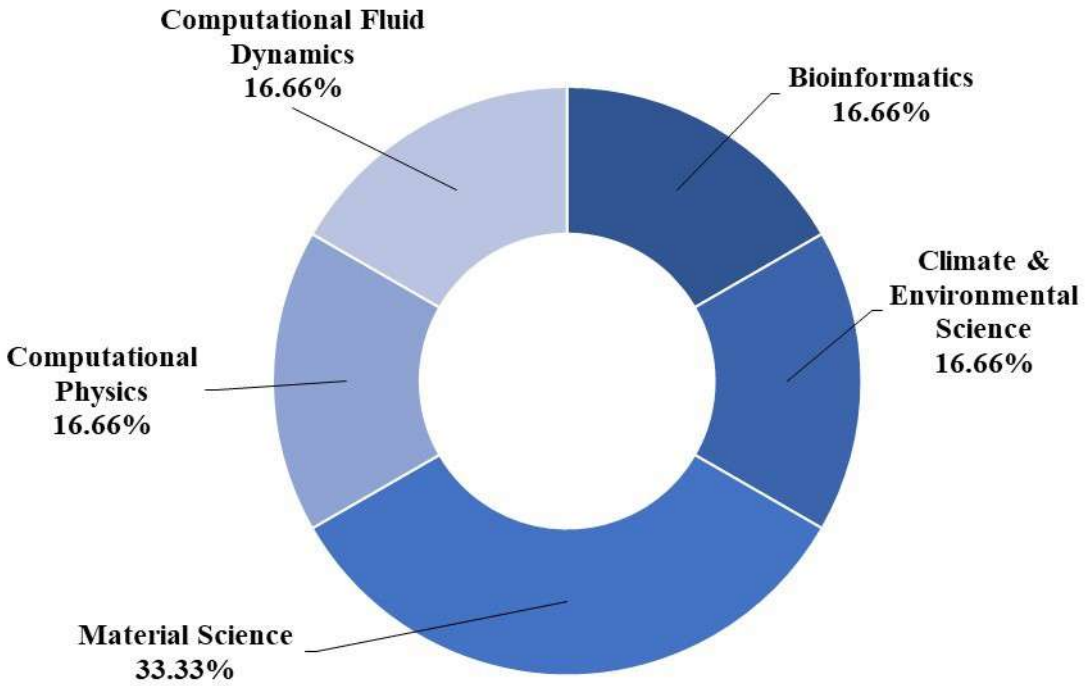


Figure: Number of PhDs across application research fields (2021)

Table: Number of PhDs across research fields

	Number of PhDs	
Application Research Fields	**Number of PhDs 2020**	**Number of PhDs 2021**
Bio Science	0	0
Chemical Science	2	0
Bioinformatics	1	1
Computational Science	1	0
Material Science	1	2
Climate & Environmental Science	0	1
Computational Physics	4	1
Computational Fluid Dynamics	1	1
Geological Science	1	0

Sectoral Usage Wise No. of projects

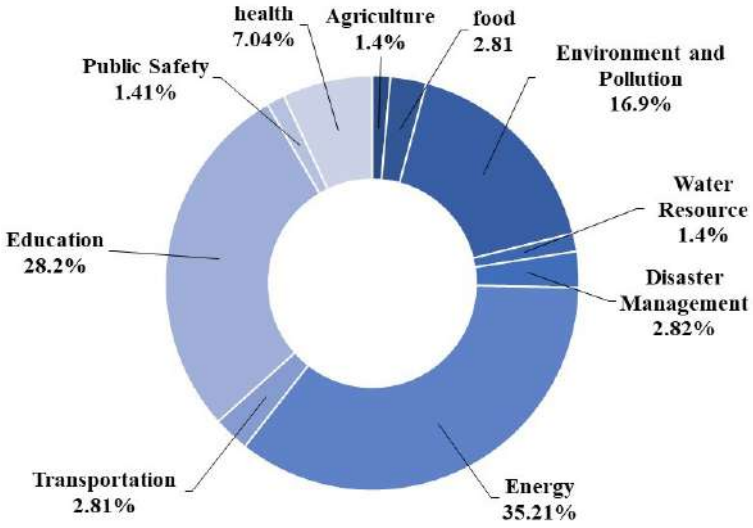


Figure: Sectoral Usage Wise No. of Projects

Table: Sectoral Usage wise distribution of projects

Key Sectors	**No. of Projects**
Agriculture	1
food	2
health	5
Water Resource	1
Environment and Pollution	12
Education	20
Transportation	2
Energy	25
Public Safety	1
Disaster Management	2

6

Science using PARAM Yuva-II

Some of the work reports and research publications in high impact journals based on the work that has been carried out on NPSF PARAM Yuva-II.

6.1 Work Report Summary

Summary of PARAM Yuva-II work report is listed in this section, whearas, details of work report are placed in **Annexure 'A'**. Please click on details link to navigate on respective work report detail.

1. "DFT based Study of Topological Insulators for Spintronics Application and organic-inorganic perovskite for Optoelectronics", by Dr. Ramesh Kumar, Assistant Professor Dept. of Physics, ramesh85@gjust.org , GJU S & T, Hisar Detail

2. "Structure and Properties of Novel Transition Metal Dichalcogenide Nanosheets", by Dr. T. J. Dhilip Kumar, dhilip@iitrpr.ac.in , Associate Professor, Department of Chemistry, IIT Ropar Detail

3. "Geospatial Information Extraction from Big Satellite Data", by Dr. Sivakumar V, , Joint Director, vsivakumar@cdac.in , C-DAC, Pune Detail

4. "Conformational Dynamics of Intrinsically Disordered and Ordered Protein", Dr. Sunita Patel (DST Women Scientist), sunita.patel@cbs.ac.in, UM-DAE Centre for Excellence in Basic Sciences, Mumbai Detail

5. "Different kinds of energy conversion in 2D materials via first principles-based approach", by Prof. Dr. Abir De Sarkar, Scientist-F/Professor and Dean (Academics), abir@inst.ac.in , Institute of Nano Science and Technology, Sector-81, Knowledge City, Manauli, SAS Nagar, Mohali, Punjab - 140306 Detail

6. "Inhibitors of Plasmepsin X Plasmodium falciparum: Structure-based pharmacophore generation and molecular dynamics simulation (b) Inhibitors of Heptosyltransferase I to prevent heptose transfer against antibiotic resistance of E. coli: Energetics and stability analysis by DFT and molecular dynamics", by Malay Kumar Rana, Assistant Professor, mrana@iiserbpr.ac.in, IISER Berhampur Detail

7. "Thermoelectric behavior of KCuS monolayer", by Subhasmita Kar, PhD Scholar subhasmita1921ph02@iitp.ac.in, IIT Patna Detail

8. "Quantum_Hall-PR", by Sreejith GJ , Associate Professor, Department of Physics, anand.abhishek@stude
IISER Pune Detail

9. "Numerical simulations of hydromagnetic turbulence from galaxies to the Sun", piyali.chatterjee@iiap.res.i , Dr. Sharanya Sur, Associate professor, Indian Institute of Astrophysics Detail

10. "Dissolution of Caffeine Crystal in Supercritical CO2 Ethanol Solution", by Dr. Moumita Saharay, moumitasaharay@uohyd.ac.in , Assistant Professor, Department of Systems and Computational Biology, School of Life Sciences, University of Hyderabad, Gachibowli, Hyderabad Detail

11. "CelS-catalyzed Processive Cellulose Degradation and Cellobiose Extraction for Production ofBioethanol", by Dr. Moumita Saharay, Assistant Professor, Department of Systems and Computational Biology, School of Life Sciences, moumitasaharay@uohyd.ac.in , University of Hyderabad, Gachibowli, Hyderabad Detail

12. "Structure and Properties of Novel Transition Metal Dichalcogenide Nanosheets", Dr. Jagdish Kumar, Assistant Professor, Department of Physics and Astronomical Science, jagdish@cuhimachal.ac.in, Central University of Himachal Pradesh, Dharamshala. Detail

13. "Role of functionalised g-ZnO and g-GaN nanosheets in Optoelectronic devices: A First-principles study", by Prof. Dr. Mrinalini D. Deshpande, sandhya.wakhare@yahoo.co.in, HPT Arts and RYK Science college, Nashik, Maharashtra, India. Detail

14. "Optimizing the morphological, electric and electrochemical properties of TiO2, Polythiophene and PEDOT: PSS films and the junctions between them for use in Supercapacitors", by Prof. Ashish B. Chourasia, abchourasiansk@rediffmail.com, HPT Arts & RYK Science College, Nashik, Maharathstra Detail

15. "Study of evolution of magnetism in the defected graphene", by Prof. Anindya Datta Professor, anindya.datta@ipu.ac.in, Guru Gobind Singh Indraprastha University, New Delhi Detail

16. "RNA-Duplex" and "Ecoli_Structure", by Thenmalarchelvi Rathinavelan, Asscoiate Professor, tr@iith.ac.in, Indian Institute of Technology Hyderabad Detail

17. "First-Principle Study of the Electronic Structures of Heterostructure Devices and Their Related Applications", by Dr. Anver Aziz ,Associatet Professor , aaziz@jmi.ac.in, Jamia Millia Islamia, New Delhi Detail

18. "Computational studies on Surface enhanced Raman spectra of biomolecules adsorbed on gold and silver nanoclusters for exploration of biosensing applications", by Dr. N. V. Suresh Kumar, Assistant Professor, surshkumar_nv@vnrvjiet.in, VNR Vignana Jyothi Institute of Engineering and Technology – Hyderabad Detail

19. "Quantum_Nano-PR", by Dr. Jawar Singh, Prof. and Dean R&D, jawar@iitp.ac.in, Indian Institute of Technology Patna, Bihta, Patna Detail

20. "Time Domain Free Vibration Simulation of Bridge Deck Sections", by Dr Naresh K Chandiramani, Professor, IIT Bomabay, naresh@civil.iitb.ac.in & Dr Abhijit Gogulapati, Assistant Professor, abhijit@aero.iitb.ac.in, IIT Bombay Detail

21. "Electronic structure calculations of semiconductors", by Dr. Subrata Deb, Assistant Professor, subrata.tu@gmail.com,Women's College (Affiliated to Tripura University) Detail

22. "Photocatalytic reduction of Carbon dioxide (CO2) using Semiconductors", by Dr Aman Kaura, Assistant Professor, amankaura@pu.ac.in, Panjab University Chandigarh Detail

23. "Thermoelectric and topological Properties of novel mateirals", by Aftab Alam, Associate Proessor, aftab@iitb.ac.in, IIT Bombay Detail

24. “Simulation of Atmospheric turbulence over land”, by Prof. Abhijit Gogulapati, abhijit@aero.iitb.ac.in, IIT Bombay Detail

25. “Molecular Dynamic Simulation of Biological Macromolecules”, by Prof. Shahid M. Nayeem, msnayeem.ch@amu.ac.in , Aligarh Muslim University Detail

26. “Atomistic Modelling of Nanomaterials for Mechanical Characterization”, by Dr Rajesh Kumar, rpawar@nith.ac.in, NIT Hamirpur Detail

27. “Aerosol Radiative forcing over India (ARFI) and Atmospheric Trace Gases, Chemistry, Transport and Modelling (AT-CTM)”, by Dr. Binita Pathak, Assistant Professor, binita@dibru.ac.in, Dibrugarh UniversityDetail

28. “Computational studies on β adrenergic receptor”, by Dr. Manali Joshi, Assistant Professor, analijoshi@unipune.ac.in , S. P. Pune University Detail

29. “Electronic and thermoelectric behavior of 2D KCuSe”, by Dr.Soumya Jyoti Ray , Assistant Professor, ray@iitp.ac.in , IIT Patna Detail

30. “Computational insights into the inhibitory mechanism of peptide inhibitors against amyloid-β aggregation and protofibril destabilization”, by Dr. Deepti Goyal (Ph.D.), Assistant Professor, deepti.bansal.chem@gmail.com , Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab Detail

31. “Oxide Ion Transport in ZrO2 based Solid Electrolyte of SOFC using Molecular Dynamics simulation”, by Prof. Padma Kumar Padmanabhan, Madhual@iitg.ac.in , Indian Institute Of Technology–Guwahati Detail

32. “Study of Heusler alloys for spintronics and thermoelectric applications”, Prof. Atul Saxena, Professor, asaxena@nehu.ac.in , North-Eastern Hill University Detail

33. “Novel perovskite-based solar cells: Investigation of potential properties using ab-initio approaches”, by Dr. Yogesh Sonvane Assistant Professor, yas@phy.svnit.ac.in , Sardar Vallabhbhai National Institute of Technology Detail

34. “Atomistic Computer Simulation of Fast Ion Conducting Solids”, by Prof. Padma Kumar Padmanabhan / Professor, padmakumarp@iitg.ac.in , Indian Institute Of Technology Guwahati, Guwahati, Assam Detail

35. “Study of thermoelectric properties of bulk nanostructured materials using Monte Carlo Simulations”, by Dr. Neeleshwar Sonnathi(sn@ipu.ac.in) and Dr Anjana Bagga , USBAS, GGSIP University Detail

36. “Medical image and text data analysis using deep learning techniques”, by J.V. Bibal Benifa, Assistant Professor, benifa@iiitkottayam.ac.in , IIIT Kottayam Detail

6.2 Ph.D Theses

1. **Title of the thesis : A theoretical study of 2d boron monochalcogenide BX(X=S,Se,Te) for energy storage applications**
   Ph.D Scholar Name :Pushkar Mishra
   Name of the Supervisor : Yogesh Sonvane
   Application Research Area : Material Sciences
   Name of the Institute : Sardar Vallabhbhai National Institute of Technology, Gujarat

2. **Title of the thesis : Ab-initio study of some silicon based 2d materials for energy and sensing applications**
   Ph.D Scholar Name: Radha somaiya
   Name of the Supervisor: Yogesh Sonvane
   Application Research Area : Material Sciences
   Name of the Institute : Sardar Vallabhbhai National Institute of Technology, Gujarat

3. **Title of the thesis : Atomic Scale design of graphene based material for gas sensors : DFT study**
   Ph.D Scholar Name : Manasi Suresh Mahabal
   Name of the Supervisor: Dr. Mrs. M. D. Deshpande
   Application Research Area : Material Sciences
   Name of the Institute : Department of Physics, Savitribai Phule Pune University, Pune

4. **Title of the thesis : First Principle study of 1D Graphene Derivatives**
   Ph.D Scholar Name: Rajesh Thakur
   Name of the Supervisor: Prof. Raman Sharma
   Application Research Area : Computational Physics
   Name of the Institute: Himachal Pradesh University

5. **Title of the thesis : Two dimensional chalcogenides as promising materials for thermoelectric applications**
   Ph.D Scholar Name: Shagun Nag
   Name of the Supervisor: Ranjan kumar & Ranber singh
   Application Research Area : Computational Physics
   Name of the Institute: Panjab University

6. **Title of the thesis : Design, synthesis and evaluation of multi-target directed ligands in Alzheimer's disease treatment**
   Ph.D Scholar Name: Kamaljot Singh
   Name of the Supervisor: Dr. Deepti Goyal
   Application Research Area : Bioinformatics
   Name of the Institute: Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab

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6.3 Publications

List of publications Peer-Reviewed by NPSF PARAM Yuva-II users

Publications in National and International Journals (with their impact factor)

Following publications resulted from NPSF PARAM Yuva-II usage by its users. The publications are listed by the impact factors of the journal they are published in. The impact factor (IF) of an academic journal is a measure reflecting the average number of citations to recent articles published in the journal.

Publications 2021

1. 2D Sb2C3 monolayer: A promising material for recyclable gas sensor for environmentally toxic nitrogen-containing gases (NCGs) , V. Kumar, D. Azhikodan and D. R. Roy, Journal of Hazardous Materials (Elsevier Sci.) 405 (2021) 124168, 0304-3894, Impact Factor: 10.588
2. Electric field-induced band modulation of predicted ternary 2D MXC3 [M:X=As:Ge, Sb:Sn and Bi:Pb] with strong stability and optical properties, V. Kumar, K. Rajput and D. R. Roy, CARBON (Elsevier Sci) 172 (2021) 791-803. 0008-6223, Impact Factor: 9.594
3. Spin-Current Modulation in Hexagonal Buckled ZnTe and CdTe Monolayers for Self-Powered Flexible-Piezo-Spintronic Devices, Manish Kumar Mohanta,Fathima IS,Amal Kishore, and Abir De Sarkar*,ACS Appl. Mater. Interfaces 2021, 13, Impact Factor: 9.229
4. Effect of Dislocation Network on Precipitate Morphology and Deformation Behaviour in Maraging steels: Modelling and Experimental Validation, Kevin Jacob, Abhinav Roy, M P Gururajan and B Nagamani Jaya, Materialia 2021 , Impact Factor: 8.203
5. Ca2C MXene Monolayer as A Superior Anode for Metal-Ion Batteries, K. Rajput, V. Kumar, T. Siby, M. A. Zaeem and D. R. Roy, 2D Materials (Inst. Of Phys.) 8 (2021) 035015, 2053-1583, SCI Impact Factor: 7.103
6. A Core–Valence Separated Similarity Transformed EOM-CCSD Method for Core-Excitation Spectra, Ranga, S., & Dutta, A. K., Journal of Chemical Theory and Computation, 17, 7428–7446, (2021). Impact Factor: 6.80
7. Dissociation of air pollutants on the uniform surface of pentagonal BeP2," K. Lakhani et al., Applied Surface Science, vol. 570. Elsevier BV, p. 151061, Dec. 2021.Impact factor:6.7
8. Doorway mechanism for Electron Attachment Induced DNA Strand Break, Narayanan S J, J., Tripathi, D., & Dutta, A. K., Journal of Physical Chemistry Letters, 12, 10380–10387, (2021). Impact Factor: 6.42
9. "Inhibitors of Plasmepsin X Plasmodium falciparum: Structure-based pharmacophore generation and molecular dynamics simulation", Panda, S. K., Saxena, S., Sen Gupta, P. S. & Rana, M. K., Journal of Molecular Liquids, 116851, 2021, Impact Factor: 6.165
10. Carbon Nitride Monolayers as Efficient Immobilizers toward Lithium Selenides: Potential Applications in Lithium–Selenium Batteries, Swapnil S. Deshpande, Mrinalini D. Deshpande, Khidhir Alhameedi, Rajeev Ahuja, and Tanveer Hussain, ACS Appl. Energy Mater. 2021, 4, 4, 3891–3904 Impact factor:6.024

11. Potential SiX (X = N, P, As, Sb, Bi) homo-bilayers for visible-light photocatalyst applications, Radha N Somaiya, Deobrat Singh, Yogesh Sonvane, Sanjeev K. Gupta and Rajeev Ahuja, RSC Catalysis Science & Technology, 11, 4996 (2021)Impact factor: 5.721

12. First Principles Calculations of SiBi Nanosheets as Sensors for Oxygen-Containing Gases, V. Kumar, A. Bano and D. R. Roy, ACS Applied Nano Materials (Am. Chem. Soc.) 4 (2021) 2440–2451, 2574-0970,SCI Impact Factor: 5.097

13. Master Blaster: an approach to sensitive identification of remotely related proteins, Chintalapati Janaki, Venkatraman S. Gowri & Narayanaswamy Srinivasan, Scientific Reports volume 11, Article number: 8746, 2021, Impact Factor: 4.38

14. Role of Framework Flexibility in Ion Transport: A Molecular Dynamics Study of LiMIV2(PO)4", Krishnanjan Pramanik, Kartik Sau and P. Padma Kumar, J. Phys. Chem. C, 124, 4001-4009 (2020), Impact Factor:4.126

15. Phase field modelling of morphologies driven by tetragonal interfacial energy anisotropy, Arijit Roy and M P Gururajan, Crystal Growth & Design, Vol 21 (3), 1591-1603, 2021. (ACS Editors' Choice article) , Impact Factor : 4.076

16. An efficient Fock space multi-reference coupled cluster method based on natural orbitals: Theory, implementation, and benchmark, Haldar, S., & Dutta, A. K., Journal of Chemical Physics, 155, 014105 (2021). Impact Factor: 3.99

17. A similarity transformed second-order approximate coupled cluster method for the excited states: Theory, implementation, and benchmark, Haldar, S., Mukhopadhyay, T., & Dutta, A. K., Journal of Chemical Physics, 156, 014110. Impact Factor: 3.99

18. Electronic and optical properties of boron-based hybrid monolayers, Katoch, N., Kumar, A., Kumar, J., Ahluwalia, P. K. & Pandey, R., Nanotechnology, 32, 415203, 2021. Impact Factor: 3.87

19. Hydrogen-Induced Tunable Electronic and Optical Properties of Two-Dimensional Penta-Pt2N4 Monolayer , V. Kumar, A. Dey, S. Thomas, M. A. Zaeem and D. R. Roy, Physical Chemistry Chemical Physics (Royal Soc. Chem.) 23 (2021) 10409-10417, SCI Impact Factor: 3.676

20. Stability and electronic properties of bilayer graphene spirals, R Thakur, PK Ahluwalia, A Kumar, R Sharma Physica E: Low dimensional Systems and Nanostructures 129, 114638, Impact Factor: 3.5

21. The interaction of two-dimensional P2SiS nanosheet with environmental toxic NCG molecules for sensor application: A DFT study ,V. Kumar, A. Bano, K. Rajput and D. R Roy, Sensors and Actuators: A. Physical (Elsevier Sci.) 322 (2021) 112608. , ISSN: 0924-4247, SCI Impact Factor: 3.407

22. Strain-induced electronic, stability and enhancement of thermoelectric performance of 2D Si2C3 monolayer: An emerging renewable energy , V. Kumar and D. R. Roy, Physica E (Elsevier Science) 132 (2021) 114769, 1386-9477, Impact Factor: 3.382

23. Influence of vacancy defects on the thermoelectric performance of SnSe sheet, S. Nag, A. Saini, R. Singh, and R. Kumar, Physica E: Low Dimens. Syst. Nanostruct., 134 (2021) 114814, Impact Factor: 3.38

24. Deformation behaviour of Cu and Cu-Al in the dislocation starved regime: a molecular dynamics study, G Kamalakshi, Prita Pant and M P Gururajan, Computational Materials Science (2021), Impact Factor: 3.3

25. "Inhibitors of Heptosyltransferase I to prevent heptose transfer against antibiotic resistance of E. coli: Energetics and stability analysis by DFT and molecular dynamics", Bhattacharya, U., Panda, S. K., Sen Gupta, P. S. & Rana, M. K., Journal of Molecular Structure, 1253, 132258, 2022, Impact Factor: 3.196

26. Electron Correlation Trends in Permanent Electric-Dipole Moments of Alkaline-Earth Metal Monohydrides", N. M. Fazil, V. S. Prasannaa, K. V. P. Latha, M. Abe , PHYSICAL REVIEW A , Impact Factor : 3.14

27. RaH as a potential candidate for electron electric-dipole-moment searches", N. M. Fazil, V. S. Prasannaa, K. V. P. Latha,,M. Abe, and B. P. Das, PHYSICAL REVIEW A 99, 052502 (2019), Impact Factor : 3.14

28. Ultrathin Pd and Pt nanowires for potential applications as hydrogen economy,Shivam Kansara, Sanjeev K.Gupta, Yogesh Sonvane, P.N.Gajjar, Material Today Communication, 26, 101761 (2021) Impact Factor: 2.768

29. Electron Attachment to Cytosine: The Role of Water, Verma, P., Ghosh, D., & Dutta, A. K., Journal of Physical Chemistry A, 125, 4683–4694, (2021). Impact Factor: 2.65

30. Phase-field study of surface diffusion enhanced break-ups of nanowire junctions, Abhinav Roy, Arjun Varma R, M P Gururajan, Journal of Applied Physics, Volume 130, 194301 (20 pages), 2021, Impact Factor: 2.546

31. Fully discrete least-squares spectral element method for parabolic interface problems, Kishore Kumar, N., Biswas, P., MATHEMATICS AND COMPUTERS IN SIMULATION, 181, 364-379, 2021 Impact Factor: 2.463

32. Exceptionally high open circuit thermoelectric figure of merit in two-dimensional Tin Sulphide, S. Nag, R. Singh, and R. Kumar, J. Condens. Matter Phys., 33 (2021) 315705, Impact factor: 2.3

33. Van der waals SiSe2 homo-bilayers for optoelectronics applications,Radha N Somaiya, Yogesh Sonvane,Sanjeev K.Gupta, Superlattices and Microstructures, 152, 106858 (2021) Impact factor: 2.120

34. Exploring the transport and optoelectronic properties of silicon diselenide monolayer, Radha N Somaiya, Yogesh Sonvane,Sanjeev K.Gupta, Superlattices and Microstructures, 150, 106813 (2021)Impact factor: 2.120

35. Geospatial Information Extraction from Big Satellite Data using CUDA-enabled GPU Parallel Computing Technique, Sivakumar V., Ankit. G., Biju C., Journal of Geomatics, 15 (2), 152-159, 2021, Impact Factor: 0.133

7

Appendix

7.1 Appendix 'A' PARAM Siddhi-AI : Detail Work Report

Work Report 1 Summary

Title of the work carried out: Bahubhashak Pilot: Development and Deployment of English-Marathi-English Machine Translation System along with Creation of Robust Evaluation System

Name & Designation of the Chief Investigator: Prof. Pushpak Bhattacharyya, Professor,Department of Computer Science and Engineering

E-mail Id:pb@cse.iitb.ac.in

Institution Name: Indian Institute of Technology, Bombay

Application Domain: Conversational AI

Research Challenge/s:

1. Train a robust machine translation system for translation between English and Marathi languages.
2. We follow a deep learning based technique (Neural Machine Translation) which is the current state-of-the-art for developing Machine Translation systems. A supervised NMT system development involves training a large neural network, containing a huge number of parameters, using a massive amount of data. This process of learning a huge number of parameters by processing vast amounts of data is time consuming and highly computationally intensive as well.

Work carried, Milestone, Achievements & Graphs, Plots:

1. Trained Neural Machine Translation Models for language directions involving English, Marathi and Hindi languages.

2. The NMT models were made available on Bhashini Platform for people to use. bhashini.gov.in

Benefits & experience of using NPSF:

The NPSF PARAM Siddhi-AI system gave access to a high number of GPUs with large amounts of GPU memory. This allowed us to run more experiments in parallel. The large amount of GPU memory allowed us to train larger size models with a high number of parameters. As the GPUs were fast it reduced the time for training the system which increased the speed of experimentation.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work :NA

Work Report 2 Summary

Title of the work carried out:A Novel Scalable High-Performance Machine Learning Algorithms for NGS Analysis of Genomics Data at Exascale Level

Name & Designation of the Chief Investigator: Dr. Aruna Tiwari, Professor, Computer Science & Engineering, IIT Indore

E-mail Id:artiwari@iiti.ac.in

Institution Name: Indian Institute of Technology, Indore

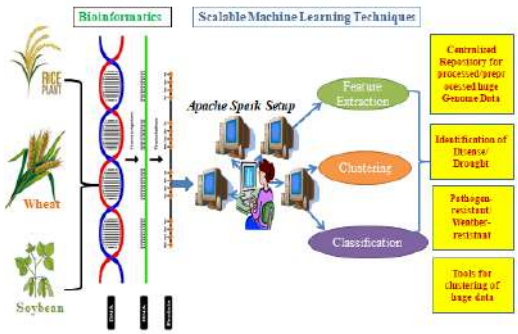
Application Domain: Big Data Analytics

Research Challenge/s:

1. To develop novel scalable hybrid machine learning algorithms using big data analytical framework for data preprocessing, feature extraction and reduction on HPC machine.
2. To perform the large-scale comparative analysis on the genomics database of different varieties our study aims to use the HPC and NSM supercomputing facility for the storage and computational processing of Wheat, Rice, and Soybean Genome data.
3. Our study aims to develop the pipelined prototype model and tools that will be deployed in the repository of NSM supported infrastructure.

Work carried, Milestone, Achievements & Graphs, Plots:

1. Preprocessing of huge genome data is performed using developed scalable feature extraction techniques on the NPSF PARAM Siddhi-AI system.
2. Clustering of huge benchmark datasets and genome datasets using developed scalable fuzzy clustering algorithms has been performed and their results are compared.
3. We have developed two scalable fuzzy clustering algorithms on the NPSF PARAM Siddhi-AI system and tested huge benchmark datasets on it.



Benefits & experience of using NPSF:

PARAM Siddhi-AI system usage has helped me in my research work. As we are working on Big Data analytics, it executes the code in less amount of time. The working environment is easy as submission of one script file can run a complete dataset for the number of subsets. The benefits and work experience are as follows:

1. We have successfully pre-processed genome data using our developed code.
2. We have used multiple nodes for clustering and subset division and it is working fine.
3. We can submit multiple jobs in a single script file that is not possible for normal spark clusters.
4. We have clustered big datasets in less amount of time.

Analysis of run-time on PARAM Siddhi-AI system: The datasets we have evaluated and clustered on PARAM Siddhi-AI system took only 1 hr for complete pipeline and testing. The same datasets on normal cluster setup of commodity hardware take 36 hr for a complete evaluation. Thus, the pipeline of our project for the work we have completed so far has been successfully set-up.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : The helpdesk has responded with great promptitude in installing different programs & modules required by us from time to time. In short, helpdesk has been remarkably supportive. We owe the deepest debt of gratitude to CDAC-Pune and the support team of PARAM Siddhi-AI system. The support team's response is fast and always helped us in time.

Work Report 3 Summary

Title of the work carried out: The numerical investigation of natural convection phenomena in the simple/complex porous media using deep learning techniques

Name & Designation of the Chief Investigator: Dr. S.V.S.S.N.V.G. Krishna Murthy

E-mail Id: skmurthy@diat.ac.in

Institution Name: Defence Institute of Advanced Technology, Pune

Application Domain: Computational Fluid Dynamics

Research Challenge/s: The access to the PARAM-Siddhi Computing facility was given in the month of November, and the computational environment (Tensorflow and Cuda version) was not managed according to our requirement. However, the support team is very active and helpful in nature, whose positive response and better response make it to install an alternate computational environment. It took me almost 2.5 months to configure it, and now I could run my code on the compute node efficiently.

Work carried, Milestone, Achievements & Graphs, Plots:

We are implementing a deep learning technique to solve the complex physical phenomena in the case of natural convection in the 3D porous enclosure.Only a testing case has been compiled on a single compute node. From now onward, we will execute the code and compute it on it.

Benefits & experience of using NPSF:

Our research problem is based on the numerical solution of a simple and complex mathematical model for natural convection phenomena in 2D/3D porous enclosures. We have successfully solved a simple 2d problem using deep learning techniques on our local machine, but a huge amount of time was required in the study of a 3D model with complex physics embedded in it. To overcome the computational difficulties, we have chosen the PARAM siddhiAI system that is working efficiently in our research case.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work :

I want to extend my thankful note to the support team of NPSF PARAM Siddhi-AI. The entire support team is very supportive and capable of handling the issue efficiently. I am very much fascinated with the computational capability of the present set-up of NPSF PARAM Siddhi and its support team.
I want to add a small remark to the current working environment is that to please add some extra CUDA toolkits for the compatibility of the older version of TensorFlow version-1.15.

Work Report 4 Summary

Title of the work carried out: Design and Development of Quantum Computing Toolkit (simulator and workbench) and capacity building

Name & Designation of the Chief Investigator: Lakshmi Eswari P R, Director, C-DAC Hyderabad

E-mail Id: prleswari@cdac.in

Institution Name:C-DAC Hyderabad

Application Domain: Quantum Computing

Research Challenge/s: Benchmarking of the indigenously developed Quantum Computer Simulator QSim.Finding out number of Qubits supported by QSim

Work carried, Milestone, Achievements & Graphs, Plots:

QSim is country's first quantum computer simulator toolkit and it was Launched on 27th August 2021, and has enable researchers and students to carry out cost-effective research in quantum computing. Initial deployment of QSim was made on PARAM SIDDHI AI NODE.
QSim can be accessed at https://qctoolkit.in QSim allows researchers and students to write and debug Quantum Code that is essential for developing Quantum Algorithms.
The benchmarking of the Simulator QSim was done on the Single Node , and experiments were performed to find out max Qubits supported by QSim for the benchmark with runtime under two hours.

Benefits & experience of using NPSF:

Local machines on which we were benchmarking QSim were constrained and had limited resources, PARAM Siddhi-AI system helped us to provide the HPC configuration necessary for carrying out benchmarking of QSim and figuring out the current limit of Qubits that the QSim supports. It has helped us to figure out limitation and the bottlenecks associated with the QSim. Helped in gaining the knowledge of the HPC workflow that made possible for us to integrate QSim to systems like PARAM SHAKTI. Currently QSim runs on cloud environment backed up by powerful HPC resources.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Siddhi-AI for your research work :It provided the right kind of environment for carrying out benchmarking/experiments using QSim.

Work Report 5 Summary

Title of the work carried out: Early warning system for flood prediction in river basins of India

Name & Designation of the Chief Investigator: Ms. Upasana Dutta, Joint Director

E-mail Id:upasanad@cdac.in

Institution Name:C-DAC Pune

Application Domain: Hydrological Sciences

Research Challenge/s:

1. GPU code of Anuga is not available
2. Tried to run job across nodes but libraries were not accessible on other nodes hence it failed
3. Hyper-threading on single node could not increase the performance

Work carried, Milestone, Achievements & Graphs, Plots:

1. Setting up environment and installation of required libraries
2. We could successfully run delta simulation on single node
3. Experimented with hyper-threading

Benefits & experience of using NPSF:

NA

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Siddhi-AI for your research work :It would be helpful if we can get multi-nodes to execute our model

Work Report 6 Summary

Title of the work carried out:A high-performance, scalable FFT library & Pseudo-spectral code (Tarang) for modern GPUs

Name & Designation of the Chief Investigator: Mahendra K. Verma, Professor

E-mail Id:mkv@iitk.ac.in

Institution Name: IIT Kanpur

Application Domain: Computational Fluid Dynamics

Research Challenge/s: In general turbulence simulation by the use of spectral method requires a lot of FFT usage, which becomes a bottleneck for larger grid sizes. So, GPU based FFT and a pseudo-spectral solver will be helpful to preform turbulence simulation for larger grid sizes. We faced some issues while using GPU -Direct RDMA during multi-node communications.

Work carried, Milestone, Achievements & Graphs, Plots:

I worked with Soumyadeep Chatterjee, under the guidance of Prof. Mahendra K. Verma on this project. We made our own multi-node FFT GPU library using Nvidia's cuFFT library and Open-MPI. We are now porting our Pseudo-spectral code Tarang on GPUs using PARAM-Siddhi-AI system. We are also going submit a paper on our multi-node FFT to Journal of Parallel and distributed computing (JPDC).

Benefits & experience of using NPSF:

While developing our application, initial phase of testing and optimizations are done on Param-Siddhi AI. In our own custom CUDA kernels for matrix transpose we were able to achieve bandwidth as near as 97% of a simple copy kernel.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Siddhi-AI for your research work :It was great experience while working on such a highly prestigious supercomputer. Hope we will be able to get more out of this system for our Research work. It will be helpful if all the nodes are up as soon as possible which will help us to scale our GPU based Pseudo-spectral code on multi-node and multi-GPUs.

Work Report 7 Summary

Title of the work carried out: qttransport

Name & Designation of the Chief Investigator: Dr. Jawar Singh, Prof. and Dean R&D

E-mail Id:jawar@ iitp.ac.in

Institution Name: Indian Institute of Technology, Patna

Application Domain: Material Sciences and Computational Physics

Research Challenge/s: According to the IRDs road map, the gate length of MOSFETs cannot be reduced beyond 12nm. This contradicts Denard's scaling theory that acts as a guideline to the semiconductor industry to miniaturize MOS technology in order to comply with Moore's Law. Thus it limits the usage of conventional materials in future device technologies. These issues motivated us to investigate 2D materials for future device applications like sensing, MOSFETs, spintronics, etc. because it is observed experimentally that 2D materials show far better electrostatics when compared to conventional 3D counterparts.

Work carried, Milestone, Achievements & Graphs, Plots:

Our account on PARAM Siddhi was created last month therefore it will take some time to perform research.

Benefits & experience of using NPSF:

NA

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Siddhi-AI for your research work : NA

Work Report 8 Summary

Title of the work carried out: Monocular depth estimation using multi scale transformer

Name & Designation of the Chief Investigator: Ashutosh Agarwal (Student)

E-mail Id: csy202452@iitd.ac.in

Institution Name: Indian Institute of Technology, Delhi

Application Domain: N/A

Research Challenge/s: N/A

Work carried, Milestone, Achievements & Graphs, Plots: N/A

Benefits & experience of using NPSF: N/A

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : N/A

Work Report 9 Summary

Title of the work carried out: PSA Bahubhashak Pilot

Name & Designation of the Chief Investigator: Dipti Misra Sharma, Professor

E-mail Id: dipti@iiit.ac.in

Institution Name:IIIT-Hyderabad

Application Domain: Conversational AI

Research Challenge/s: High end models like NMT systems requires heavy computations and thorough experimentation. Sometimes when the servers are down, it become difficult to train the models from the scratch.

Work carried, Milestone, Achievements & Graphs, Plots:

Developed Machine Translation Systems used for domains like AI/Programming, Health

Benefits & experience of using NPSF:

Yes, availability of GPUs for training NMT systems helped me to build multiple models and analyze them for further improvements.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Siddhi-AI for your research work : Some backup servers would be useful for training models.

Title of the work carried out: Adapt2Adverse: Improving Domain Generalization in Urban-Scene Segmentation in Adverse Weather Conditions

Name & Designation of the Chief Investigator: Dr. Chetan Arora, Associate Professor

E-mail Id: chetan@cse.iitd.ac.in

Institution Name:IIT-Delhi

Application Domain: Computer Vision

Research Challenge/s: It would be helpful if software and packages like Matlab, TensorFlow, PyTorch, etc. are provided as modules to load directly.

Work carried, Milestone, Achievements & Graphs, Plots:

Proposed work: Semantic segmentation of adverse weather images is a challenging task in computer vision with many real-world applications such as autonomous navigation. State-of-the-art (SOTA) methods trained on broad daylight images undergo severe performance degradation due to the illumination shift from daylight to adverse weather images. On the other hand, SOTA techniques rely on accessing the source data or its auxiliary information (e.g., GPS) to transfer knowledge from daylight to adverse weather images. Moreover, they perform poorly on segmenting the small objects (e.g., traffic lights) or large monotonic regions (e.g., sky, road). To remedy this, we propose a full test time adaptation framework, namely Adapt2Adverse, which learns to generalize on unseen adverse weather images during inference. More specifically, given a pre-trained model and its parameters, our method enforces edge consistency prior to the inference stage and updates the model based on a single test sample at a time (Adapt2Adverse-sample) or continuously for the whole test domain (Adapt2Adverse-domain). Adapt2Adverse framework does not need access to the source data and can be used for any pre-trained model. We demonstrate that given a model pre-trained on daylight images, the Adapt2Adverse framework outperforms adverse weather image segmentation methods, both in domain generalization and test-time adaptation settings. We further show that the edge consistency prior is effective, even if the model is pre-trained on adverse weather images. We apply Adapt2Adverse to adverse visual conditions such as fog, snow, night, cloudy, overcast, and rain to demonstrate the target domain-agnostic effectiveness of the proposed approach. **Societal Impact:** Out-of-domain generalization plays a pivotal role in the success of deep neural networks for safety-critical applications such as autonomous navigation. Although DNNs based architectures have achieved tremendous success in many computer vision tasks, they don't perform well when the test data comes from a domain with different sample distribution, referred to as the domain shift. Domain shift can be caused by different factors such as input corruption, adverse weather (rain, snow, etc.), illumination changes (e.g. nighttime), adversarial attacks, or even sensor malfunction. Ensuring robust performance on unseen target domains is critical for the real-world applicability of deep neural networks in Autonomous navigation.

Benefits & experience of using NPSF:

NPSF PARAM Siddhi-AI system helped my research work to scale the experiments to large-scale

datasets. NPSF PARAM Siddhi-AI helps to perform experiments on computer heavy architectures like Transformers.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : NA

Work Report 11 Summary

Title of the work carried out: Deep Learning Algorithms like Convolutional Neural Networks

Name & Designation of the Chief Investigator: Dr. Manjari Gupta, Associate Professor

E-mail Id: manjari@bhu.ac.in

Institution Name: Banaras Hindu University(BHU), Varanasi

Application Domain: Computer Vision

Research Challenge/s: Unable to use sudo privileges

Work carried, Milestone, Achievements & Graphs, Plots:

Execution of 2D CNN code on CIFAR dataset

Benefits & experience of using NPSF:

NA

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Siddhi-AI for your research work : NA

Work Report 12 Summary

Title of the work carried out: Emotion recognition and Classification of Humans, Using EEG signals from the Dataset: GAMEEMO

Name & Designation of the Chief Investigator: Dr. Manjari Gupta, Associate Professor

E-mail Id: manjari@bhu.ac.in

Institution Name: Banaras Hindu University(BHU), Varanasi

Application Domain: Cognitive sciences

Research Challenge/s: NA

Work carried, Milestone, Achievements & Graphs, Plots:

We applied various Signal processing techniques and Transformations such as Discrete Wavelet Transform (DWT), Continues wavelet Transform (CWT) Wavelet Scattering Transform (WST) etc., on EEG signals. Then we applied machine learning and deep learning methods to classify the emotions. We are writing a Research Paper which we soon will complete.

Benefits & experience of using NPSF:

NPSF PARAM Siddhi-AI helped a lot in my research work. The computations which I need to be carry out were not working in my personal PC, I tried google colab also but the system got crashed when I was running the code on colab. By using Siddhi-AI our code has run faster and execution time has reduced drastically.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work :
It was a wonderful experience working with the India's fastest Super computer

Work Report 13 Summary

Title of the work carried out: Automatic Speech Recognition in Indian English, Tamil, Hindi, and Text to Speech Synthesis for conversational speech in Indian languages, in particular Hindi, Tamil, and Indian English

Name & Designation of the Chief Investigator: Hema A Murthy, Professor

E-mail Id: hema@cse.iitm.ac.in

Institution Name:IIT Madras

Application Domain: Conversational AI

Research Challenge/s:

1. Models trained on A100 GPUs were not working on other GPUs
2. Waiting times for resources were long

Work carried, Milestone, Achievements & Graphs, Plots:

1. Training bi-lingual text-to-speech end-to-end models for Tamil+English.
2. Training Waveglow vocoder using multi-lingual data.
3. Training Tacotron2 based architecture for multilingual TTS systems.
4. Trying out new architectures for training TTS systems.
5. Star GAN and Cycle GAN experiments for voice conversion.
6. Bilingual voice training for Bengali end-to-end TTS voices.

Benefits & experience of using NPSF:

We are able to try out various experiments, which were earlier restricted due to resources.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work :

1. Please give an option to only acquire CPUs without the allocation of GPUs.
2. The training speeds reduce significantly while using multiple nodes compared to using a single node. This may be due to the data transfer bottleneck between nodes. Please address this issue.
3. Limit the number of bash terminals allocated to users, since resources don't get reallocated after running, when a user is executing codes after acquiring a terminal.

Work Report 14 Summary

Title of the work carried out: IndicASR -Automatic Speech Recognition Models for Indian Languages

Name & Designation of the Chief Investigator: Mitesh M. Khapra, Associate Professor

E-mail Id: miteshk@cse.iitm.ac.in

Institution Name:IIT Madras

Application Domain: Conversational AI

Research Challenge/s:

1. India has over a billion speakers collectively speaking over 100 languages. Building high-quality ASR models for such a large and diverse pool of languages is challenging, even if we restrict ourselves to top-30 largely spoken languages.
2. Many modern ASR models rely on large amounts of labeled data for each language to build high-quality ASR systems. Such approaches are expensive and not scalable, thus limiting the reach of ASR technologies to some languages and a section of the population.
3. In addition to these challenges on availability of labeled data, Indian languages also face a lot of challenges due to larger character set, agglutinative nature of the languages etc.
4. We study the impact of multilingual pretraining to reduce the dependency on labeled data.

Work carried, Milestone, Achievements & Graphs, Plots:

1. Training large models comes with the overhead of collecting and processing huge amounts of unlabelled corpus. Curating and pre-processing datasets of TB order requires huge amount of compute and PARAM Siddhi-AI system helped us scale easily
2. We trained large Language Models of order hundreds of Million parameters. With the multi-node-multi-GPU setup we were able to perform experiments at a significantly faster rate
3. We have curated the largest speech corpus with 17k hours of data covering 40 Indian languages
4. In this work we focus on building Speech Recognition models for Indian languages, we also ablate on different components that impact the performance of the model
5. We have created state-of-the-art Speech Recognition Models for 9 Indian languages
6. The work is published at AAAI 2022 and will be presented at the conference in Feb 2022- Towards Building ASR Systems for the Next Billion Users
7. We have open sourced all our data and models for public usage - https://indicnlp.ai4bharat.org/indicwav2vec/

Social Impact:

Our code, data and models are available publicly and we hope they will help advance research in ASR for Indic languages. Our open-sourced models can impact small-scale startups and individuals to enable speech recognition services/applications for Indian languages with low barriers to expertise and resources.

Publication:

Towards Building ASR Systems for the Next Billion Users, T. Javed, S. Doddapaneni, A.Raman, K. Bhogale, G. Ramesh, A. Kunchukuttan, P. Kumar, M. Khapra. Thirty-Sixth AAAI Conference on Artificial Intelligence **Results:**

Table : Result

	gu	ta	te
Baseline	**19.8**	**19.4**	**22.6**
Jilebi	14.0	13.9	14.7
Cogknit	17.7	16.0	17.1
CSALT-LEAP	-	16.3	17.6
ISI-Billa	19.3	19.6	20.9
MTL-SOL	18.4	16.3	18.6
Reed	16.1	19.9	20.2
CNN+ContextTemporal Feat.	18.4	24.3	25.2
Reed	16.1	19.9	20.2
EkSetp	19.5	22.1	21.9
Our Best Model	**11.7**	**13.6**	**11.0**

Benefits & experience of using NPSF:

The models we pretrain are quite huge with orders of a few hundred millions of parameters and the dataset size grows to order billion samples. NPSF PARAM Siddhi-AI system has made it possible for us to train such huge models with ease by leveraging the Multi-Node-Multi-GPU setup. With each node having 256 cores with 1TB of data, data processing is extremely fast when we use all the cores in the node. This setup has made us scale to larger models and datasets with ease. The large capacity network storage in the system has allowed us to work with large datasets conveniently.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work :

1. NPSF Helpdesk is very prompt in their replies with any of our queries. They helped us sort of many issues very quickly
2. Monitoring of nodes and utilization can be made better
3. Some workflows require us to access the internet to upload logs, currently we write to offline files and upload them from login-node. Other alternatives would be helpful

Title of the work carried out: Hours to Milliseconds:Leveraging machine learning methods to reduce the computation time for crop yield prediction

Name & Designation of the Chief Investigator: Prof. Ganti S. Murthy, Professor

E-mail Id: Ganti.murthy@iiti.ac.in

Institution Name: Indian Institute of Technology Indore

Application Domain: Machine learning

Research Challenge/s: None as yet. We have a prototype code that we have developed and used it on PCs. We will be scaling it for use on the HPC.

Work carried, Milestone, Achievements & Graphs, Plots: We are yet to use the system. Our project staff has left and we are recruiting new project fellow.

Benefits & experience of using NPSF:

NA

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : As a first time user, the manual provided by the PARAM Siddhi team was very valuable to understand the HPC usage.

Work Report 16 Summary

Title of the work carried out: Sign Language Accessibility for e-Governance Services

Name & Designation of the Chief Investigator: Balan C, Senior Direct

E-mail Id:cbalan@cdac.in

Institution Name: Center for Development of Advanced Computing

Application Domain: Computer Vision

Research Challenge/s: Developing a robust and accurate product level Machine Learning solutions for sign language recognition is challenging task. We are trying out the state-of-the-art deep learning-based solutions for the same which requires HPC machines for training.

Work carried, Milestone, Achievements & Graphs, Plots:

Analysis of Machine Learning models on ISL dataset. Work in-progress. This application will provide a interface for accessibility to E-Governance services for deaf community proficient in ISL

Benefits & experience of using NPSF:
The system helped us to train the computationally intensive model faster, thus reducing our waiting period.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : Timely update of the user manual would have made HPC access and usage easier, thereby effectively avoiding project delay .

Work Report 17 Summary

Title of the work carried out: Bahubhashak(NMT)

Name & Designation of the Chief Investigator: Dr. Ajai Kumar, Senior Director

E-mail Id:ajai@cdac.in

Institution Name: Center for Development of Advanced Computing, Pune

Application Domain: Conversational AI

Research Challenge/s: N/A

Work carried, Milestone, Achievements & Graphs, Plots: N/A

Benefits & experience of using NPSF: N/A

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : N/A

Work Report 18 Summary

Title of the work carried out: iOncology.ai

Name & Designation of the Chief Investigator: Dr. Ajai Kumar, Senior Director

E-mail Id:ajai@cdac.in

Institution Name: Center for Development of Advanced Computing, Pune

Application Domain: AI in Oncology

Research Challenge/s: NA **Work carried, Milestone, Achievements & Graphs, Plots:**

1. DNN based Binary Classification on Breast MRI images [Completed]
2. DNN based Binary and Multi-class classification on Breast Histopathology images [completed]
3. ML based binary classification on breast mammographic mass report data[Completed]
4. ML based quality of life analysis based on ovarian cancer clinical data[Completed]

Research Activities:

Analysis on Tongue Images:

1. Multiple models based on characteristics of tongue [2 incremental levels Completed]
2. Inference from all models and exporting to excel sheet for manual analysis [Completed]
3. Building Hybrid model (detection from image+clinical parameters) based on all multiple models and clinical parameters [Completed]

Analysis on Sputum Images:

1. Based on algorithm designed (Combination of Color based Segmentation and K-Means Clustering), development of program is completed results are shared with AFMC for concordance study
2. Research paper based on experiment [Completed and published in AFMC Medical journal]
3. DNN based Approach experiment (on sample 200 images) - Completed (Poster presentation is done at ICHAMS2022 https://ichams2022.exordo.com)

Analysis on Blood Smear Cell Images for detection of malaria:

1. Classification model based on different algorithms are build and tested [Completed]

Benefits & experience of using NPSF:

1. It helped in training models by applying different AI techniques and evaluation
2. Testing of models on test dataset in bulk and exporting results to excel
3. Building models based on Tensorflow object detection techniques

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work :

As path is changing while moving to different hardware configurations we need to reinstall software's and all virtual environments which tedious and time consuming, if same path is maintained then this can be overcome.

Title of the work carried out: Quantum Simulation and Computation of Atomic and Molecular Properties

Name & Designation of the Chief Investigator: Prof. Bhanu Pratap Das, Director

E-mail Id:renu.bala@tcgcrest.org

Institution Name: Centre for Quantum Engineering, Research and Education (CQuERE), TCG CREST, Kolkata

Application Domain: Atomic and Molecular Sciences

Research Challenge/s: Our area of research is theoretical atomic and molecular physics and

quantum computing. Advancements in the experimental techniques for precision measurements obviously need sound theoretical inputs to better understand various experimental aspects and sometimes to complement the experimental results. The calculations of accurate results for structural parameters and properties of atomic and molecular systems require sophisticated many body methods such as configuration interaction, many-body perturbation theory, coupled cluster etc. and large basis sets. Such structure calculations are quite expensive computationally. We do not have computational facility in our institute however we are able to perform such calculations using PARAM Siddhi-AI.

Work carried, Milestone, Achievements & Graphs, Plots:

We have run CFOUR quantum chemistry package to perform structure calculations of molecules. In addition to that, we have run quantum chemistry calculations using qiskit and pyscf softwares.

Benefits & experience of using NPSF:

Using sophisticated many-body theories, several structure calculations have been carried out that is of great demand in the field of atomic and molecular physics/chemistry.
We are also working towards the computation of excitation energies for lighter atomic systems on a quantum simulator using quantum equation of motion implemented in the qiskit software package.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : This server is easily accessible. I have installed the required softwares on it easily however I am facing blas/lapack library issues for the installation of DIRAC software. Also, please increase the maximum run time for a single job if possible.

Work Report 20 Summary

Title of the work carried out: A HPC Software Suite for Seismic Imaging to Aid Oil & Gas Exploration

Name & Designation of the Chief Investigator: Richa Rastogi, Associate Director

E-mail Id:richar@cdac.in

Institution Name:C-DAC, Pune

Application Domain: Seismic Data Processing

About Project: SeisAcoMod2D code was used to produce seismic modelling results using 2D sub-surface earth model. The code and data are available under GPL license for public use. This SeisAcoMod2D performs acoustic wave propagation of multi-source locations for the 2D subsurface earth model using finite difference time domain modeling. 2D finite-difference time-domain modeling of acoustic wave propagation. The first-order hyperbolic velocity-stress form of the wave equation is considered for discretization. Implementation is based on classic second-order or fourth-order accurate staggered-grid stencils designed on the Cartesian coordinate system (Virieux-Levander stencil). Time derivatives are discretized with classic second-order accurate staggered-grid stencil. Absorbing boundary conditions are Perfectly-Matched Layers (PML).]

Research Challenge/s: Executing our CUDA based project and Comparing performance with different GPU Hardware.

Work carried, Milestone, Achievements & Graphs, Plots:

Performance of MPI+OpenMP+Multi GPUs(CUDA) program.

Benefits & experience of using NPSF:

Table : Result

No. of GPU (Nodes)	**Performance(in Minutes) in Siddhi A100 (40GB GPU)**	**Performance(in Minutes) in Shreshtha A400 (16GB GPU)**
1 (1 Node)	66.17	100.41
2 (1 Node)	33.10	49.23
4 (1 Node)	16.16	
8 (1 Node)	8.12	
16 (2 Nodes)	4.08	
32 (4 Nodes)	2.08	

Approximately 50% reduction in execution time as compare it with Shreshtha A400 GPU's

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : Prepare modules for different environments,

Provide Guidance for How to use OpenACC Environments, Arrange Workshop for Effective Utilization of GPU Environment

Title of the work carried out: Advanced Materials and Probiotics through Machine Learning

Name & Designation of the Chief Investigator: Saroj Kumar Nayak

E-mail Id:nayaks@itbbs.ac.in

Institution Name: Indian Institute of Technology Bhubaneswar (IIT-BBS)

Application Domain: Computational Physics/Material Sciences

Research Challenge/s: Currently we are not facing any challenges.

Work carried, Milestone, Achievements & Graphs, Plots:

Our goal was to develop and/or apply a neural network for autonomous discovery of different DNA based crystals with the help of image recognition. There are several types of object detection algorithms that can be used, but it is highly relevant to choose the model which is most suited for the given task. Therefore, multiple unique neural networks are to be analyzed and considered to train upon certain input sets to generate well generalized 'weights' which can be used to detect crystals in varied conditions.

Benefits & experience of using NPSF: In order to generate weights for a mature neural network, the model must be trained for a significant amount of time and minimize any empirical losses that can be used as a metric to determine its accuracy. The system available to us, is and will prove to be immensely useful in scaling up training on the basis of several hundred images to give an idea whether there is a linear correlation between improvement in performance and increase in training size. (A comparison of current image recognition models would quickly demonstrate one particular model's utility) As our aim is to apply machine learning over a broad range of materials for different properties, we are also looking at different ML models which have successfully demonstrated in determining other variables such as fluid permeabilities in polymers after basic size distribution of synthesized nanoparticles.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : NA

Title of the work carried out: High fidelity Simulations to capture transitional and turbulent flows in turbomachines

Name & Designation of the Chief Investigator: Dr. Nagabhushana Rao Vadlamani, Assistant Professor

E-mail Id:nrv@iitm.ac.in

Institution Name: IIT Madras

Application Domain: Computational Fluid Dynamics

Research Challenge/s: We use our in-house high order solver COMPSQUARE for the computations. It is a multi-block structured compressible flow Navier-Stokes solver which is capable of scaling on both CPUs and GPUs. After domain decomposition, each grid is assigned to a single GPU. Multi-GPU computations are carried out using MPI. Some of the challenges we faced during our computations are listed below:

1. Issues with the submission scripts
2. Long job queuing times

However, with the kind assistance of the supporting staff most of the issues were resolved.

Work carried, Milestone, Achievements & Graphs, Plots:

Computations: We have been carrying out several high-fidelity simulations to explore the dynamics of turbulent flows in turbomachines. These include characterizing the flow over gas turbine intake lip under strong crosswinds (Fig 1a), studying the efficacy of different riblet shapes towards drag reduction (Fig 1b) under pressure gradients and investigating the coupled interaction of surface roughness with the free-stream turbulence typically observed in unsteady turbomachinery environment (Fig 1c). Typically, we employ around 20-135 million grid points and have used up to 8 GPU cards for all the simulations.

a) Crosswind Aerodynamic Analysis Using Quasi 3d Ducts Flow distortion during off-design conditions poses a challenge in designing the aircraft engine intake. From an aerodynamic point of view, strong crosswinds result in uneven pressure loads on the downstream fan thereby reducing efficiency. The study was conducted to investigate the behaviour of flow over a gas turbine intake lip under crosswinds (See Fig. 1a). Simulations are carried out on a quasi-3D duct (q3D), which is more computationally economical than a full 3D intake. For low mass flow rates, the flow separates over the intake lip due to an adverse pressure gradient. With an increase in the mass flow rate, the flow overcomes the adverse pressure gradient and reattaches. With a further increase in the mass flow rate, a strong shock is encountered on the intake lip and the flow separates. At low speeds, quasi-steady simulations are used to demonstrate that the flow exhibits hysteresis. Under such conditions, as also reported in the experiments, it is possible to have multiple solutions (separated/attached flow) for the same mass flow rate passing through the engine. Flow over the intake is shown to be much more sensitive to the Reynolds number, with the higher values of Reynolds number promoting attached flow.

b) Profile loss reduction of ultra high-lift turbine blades using roughness and riblets A series of high-fidelity eddy-resolving simulations are carried out to investigate the boundary layer behaviour under stream-wise varying pressure gradients. The flow development over a flat surface is examined by employing a contoured top wall, which mimics the high-lift low-pressure turbine type blade loading. The numerical framework involving the Boundary Data Immersion Method and the stream-wise varying pressure gradient (SPG) set up is validated successfully against the available computational and experimental data. Subsequently, the efficacy of roughness in suppressing the laminar separation bubble and reducing the profile loss is demonstrated by analyzing the suction surface velocity, skin friction, averaged velocity field and various boundary layer parameters. However, the roughness induced transition increases the turbulent wetted area. An attempt is made to reduce the profile loss further by employing two different riblet shapes downstream of the roughness. With sawtooth riblets, the turbulent drag increased at the trailing edge signifying the configuration to be a drag increasing one.However, with scallop-shaped riblets, there is a significant drag reduction, of about 10%, compared to the roughness alone case. However, the boundary layer parameters such as the trailing edge momentum thickness, maximum turbulent kinetic energy and Reynolds stresses have increased over the riblet surface. This is attributed to the development of a shear layer peak which is observable from the Reynolds stresses. This implies that the riblets might be reducing the skin friction drag by increasing the thickness of the viscous sub-layer which in turn results in a reduced momentum transfer to the wall and hence a reduced wall shear. When riblets are employed over the entire suction surface, the separation bubble is suppressed completely, without the need for the roughness elements.This suggests that laminar separation bubbles may not be able to sustain over a riblet surface. Further studies under streamwise varying pressure gradients will have to be performed to understand the effects of riblet spacing and height on profile loss reduction. This work is currently under progress. Currently, the riblet height and spacing were held constant, even though they are probably not optimum values under SPGs. It remains to be seen whether an optimized riblet configuration will result in a passage loss reduction in addition to decreasing the skin friction drag.

c) Dynamics of bypass transition due to surface roughness and free stream turbulence A series of eddy-resolving simulations are carried out to study the combined effect of isolated roughness and free-stream turbulence on the boundary layer transitioning over a flat plate. An isolated roughness element of fixed height is modelled using immersed boundary method and Jarrin's synthetic eddy method is used to impose free-stream turbulence (FST) at the inlet. We have imposed pulses of FST to trigger bypass transition in contrast to the continuous forcing typically studied in the literature. For a fixed turbulence intensity and length scale, the pulsing frequency of FST is varied.
The transition onset predicted from the current simulations (based on the Re Θ, t and K/δ^*t) is in agreement with the Stripf's correlations. In particular, an envelope of transition onset points was obtained from the phase-averaged flow field, whose trends are shown to agree well with Stripf's correlation. The transition length decreased with an increase in the frequency of FST pulses. Continuous wavelet transform of an unsteady signal is used to generate a scalogram, using which the FST pulse passing, vortex shedding behind the isolated roughness element and the relaxation of the roughness induced vortices to their unperturbed state are clearly illustrated. Through iso-surfaces of Q and contour plots of the streamwise velocity fluctuations on the crossflow planes, we have discussed the key mechanisms of the interaction of the FST-induced Klebanoff streaks with the roughness-induced vortices towards triggering bypass transition. **Numerical Framework:** A high-order structured multi-block in-house solver, COMP-SQUARE, is used to carry out the simulations. We solve the 3D compressible Navier-Stokes equations in generalized curvilinear coordinates. The code is equipped with explicit finite difference schemes of up to 4th order and compact schemes of up to 6th order accuracy for computing the spatial derivatives. For time stepping, the explicit four-stage fourth-order Runge-Kutta scheme is employed. An implicit spatial filter of up to 10th order accuracy with an adjustable coefficient, (-0.5

¡ αf ¡ 0.5), can be employed to suppress any high-frequency numerical instabilities arising due to unresolved wave numbers. The solver is parallelized to scale on MPI and multi-GPU platforms and the simulations in the current work are carried out using 40 GB NVIDIA Tesla A100 GPU cards. Multiple GPUs are employed for each simulation with the communication between them established through MPI. The solver has been validated on several transitional and turbulent flows over flat plates/airfoils/intakes, etc.

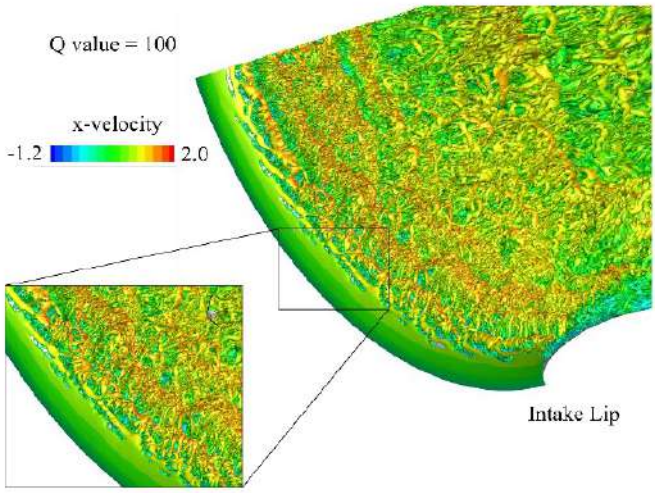


Fig. 1(a) Q-iso contour over an aero engine intake due to heavy crosswinds.

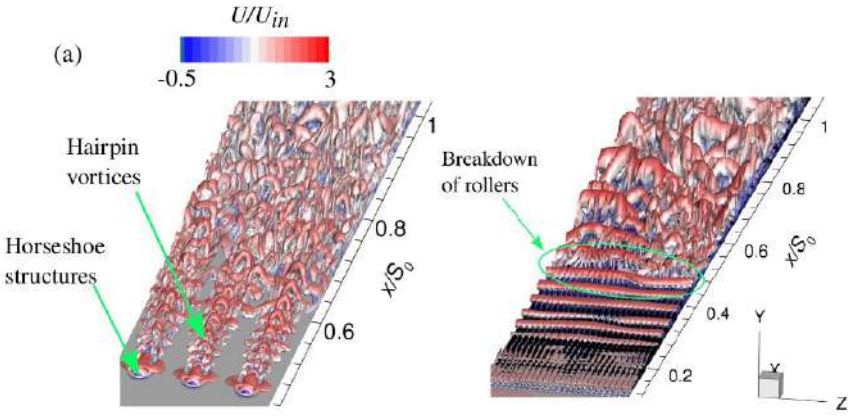


Fig. 1(b) Instantaneous iso-surfaces of Q of streamwise varying pressure gradient boundary layer in the presence of distributed roughness (left) and riblets (right)

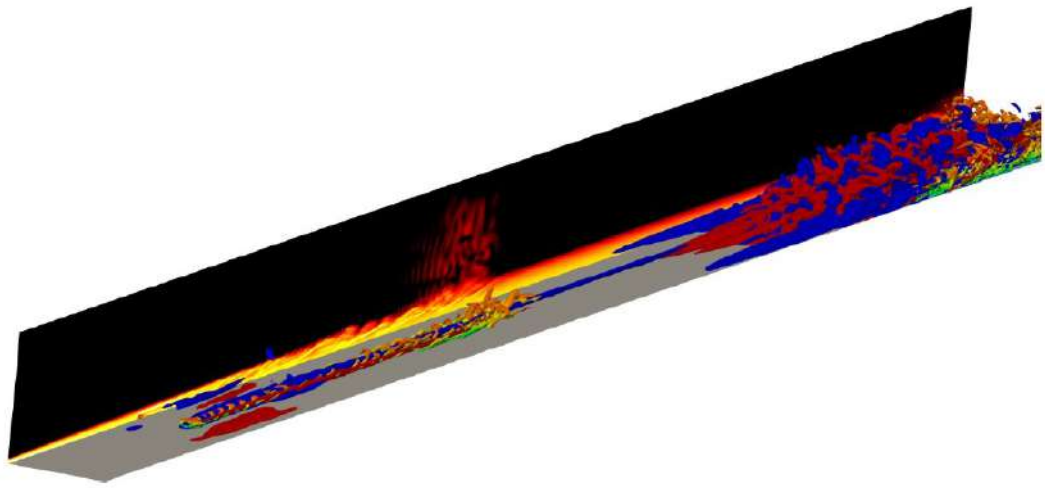


Fig. 1(c) Flow transition under the combined influence of roughness and free-stream turbulence

Solver performance and scalability: The solver was highly optimized during the GPU Hackathon events. The enhanced performance of the COMPSQUARE after the Hackathon event is as shown in Figure 2.

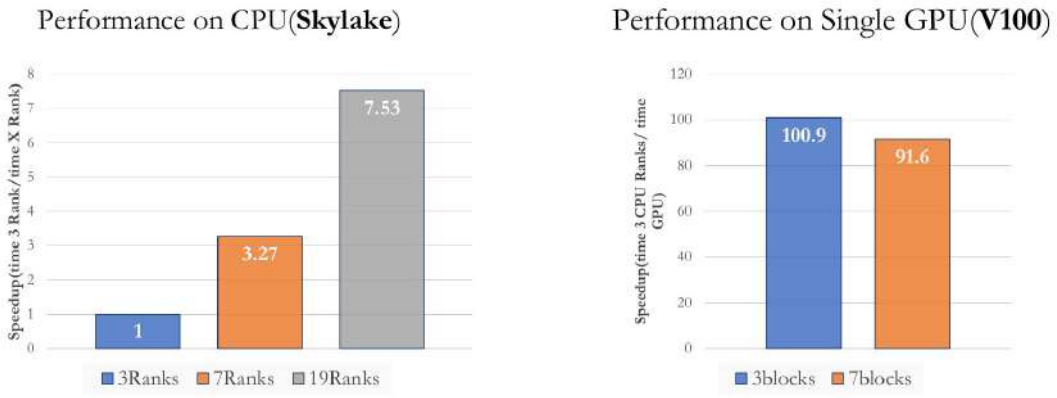


Fig. 2: Post-Hackathon performance of COMPSQUARE

textbfImpact: The outcomes from these simulations have implications for improving the understanding of complex turbulent flows. In addition, the projects are of practical relevance to the gasturbine industry. The high-fidelity data can be used to improve the low-order models typically used in the industry and subsequently design efficient gas turbine components. **Publications:**

1. "S M Ananth, Massimiliano Nardini, Aditya Vaid, Nagabhushana Rao Vadlamani, Richard Sandberg", "Profile loss reduction of high-lift turbine blades with rough and ribbed surfaces", in Proceedings of the ASME 2022 International Gas Turbine Institute & Turbomachinery Technical Conference and Exposition. , Jun 13-17, 2022 – recommended for publication in Journal of Turbomachinery. [ACCEPTED]

2. Sumit Saravankar, Adrian Arasu, Vadlamani, N. R., "Effect of Crosswind Flow on Intake Aerodynamics," in Proceedings of the ASME 2022 International Gas Turbine , Institute & Turbomachinery Technical Conference and Exposition. [ACCEPTED]

3. Sivaramakrishnan Malathi, A., Nardini, M., Vaid, A., Vadlamani, N. R., & Sandberg, R. D. (2022). On the efficacy of riblets toward drag reduction of transitional and turbulent

boundary layers. In AIAA SCITECH 2022 Forum (p. 0472) https://doi.org/10.2514/6.2022-0472

4. Vaid, A., Vadlamani, N. R., & Sivaramakrishnan Malathi, A. (2022). Dynamics of Bypass Transition with roughness and pulses of free-stream turbulence. In AIAA SCITECH 2022 Forum (p. 0453). https://arc.aiaa.org/doi/10.2514/6.2022-0453.

5. Nampelly, G., Sivaramakrishnan Malathi, A., Vadlamani, N. R., Rengarajan, S., & Kontis, K. (2022). Surface Roughness Benefits in Open Cavity Flows. In AIAA SCITECH 2022 Forum (p. 0473). https://doi.org/10.2514/6.2022-0473

Benefits & experience of using NPSF:

On the technical front, with the help of the NPSF PARAM Siddhi-AI system, we have carried out several high-fidelity numerical simulations to characterize turbulent flows in turbomachines. In particular, several parametric studies were carried out on the aforementioned topics in addition to the grid sensitivity studies. Converged turbulent statistics were recorded for all the test cases. With PARAM Siddhi system, we could significantly reduce the turnaround time to carry out these computationally intensive simulations. The outcomes from these simulations have implications for improving the understanding of complex turbulent flows. In addition, the projects are of practical relevance to the gas-turbine industry. The high-fidelity data can be used to improve the low-order models typically used in the industry and subsequently design efficient gas turbine components. On the computational front, we have seen a speedup of 2-2.5x with A100-40GB cards when compared to the V100-32GB cards. The scalability of the COMPSQUARE solver has been excellent when more GPUs are utilized for larger problem sizes. In addition, one A100 card can typically accommodate a mesh size 25-27 mil. while a V100 card can handle grids of 20-22 mil. Hence the domain decomposition can be minimized on 40 GB A100 cards. This is particularly beneficial in preserving the high order accuracy of the compact finite difference schemes. We expect the benefit to be much more on 80 GB A100 cards.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : Based on our experience with other HPC machines (at IITM and abroad), a few suggestions are given below:

1. Kindly reserve one or two nodes entirely for testing/debugging purposes whereby the users are allowed to access the same only for a short duration and not for long submissions. It is hence worth introducing a debug queue and having a separate submission script for it.

2. Once the computations are in progress, it would be helpful to grant access to the users to log in to the node and check the memory occupancy. Such login permissions are provided in the AQUA super-computing cluster of IIT Madras.

3. We hope to see the availability of A100: 80GB GPUs in the future. GPU cards with larger memory are suitable for our applications where the domain decomposition can be minimized.

Title of the work carried out: HPC GPU Applications Benchmark Results on PARAM Siddhi

Name & Designation of the Chief Investigator: Manjunatha Valmiki, C-DAC Pune

E-mail Id:manjunathav@cdac.in

Institution Name: C-DAC Pune

Application Domain: N/A

Research Challenge/s: N/A

Work carried, Milestone, Achievements & Graphs, Plots: N/A

Benefits & experience of using NPSF: N/A

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : N/A

Title of the work carried out:

1. Design, development and deployment of end-to-end speech analytics suite
2. R&D on building DNN based speech recognition system under National Supercomputing Mission (NSM)

Name & Designation of the Chief Investigator: Ajai Kumar, Senior Director, AAIG & GIST, C-DAC Pune.

E-mail Id:ajai@cdac.in

Institution Name: C-DAC Pune

Application Domain: Conversational AI

Research Challenge/s: Building of End-to-End Automatic Speech Recognition comprises many challenges, such as dealing with large speech dataset, training of acoustic model using state-of-the-art deep neural network architecture and various network topologies, fine tuning and hyper parameters optimization, accuracy improvement through different set of models and experiments etc.

Work carried, Milestone, Achievements & Graphs, Plots:

Building and training ASR models on PARAM Siddhi Compute Node

1. Building of Acoustic and Language Models using Kaldi & TDNN approaches
2. Training End2End ASR model using NeMo framework
3. Fine-tuning and Optimization of pre-train models

Deployment of ASR models on PARAM Siddhi Inference Node

1. Implement Rest services for ASR
2. Using RIVA End2End ASR pipeline
3. Optimized inference time

Development of models for speech analytics components

1. Gender Identification (GID)
2. Spoken Language Identification (SLID)
3. Speaker Identification (SID)
4. Speaker Diarization (SD)
5. Keyword Spotting (KWS)

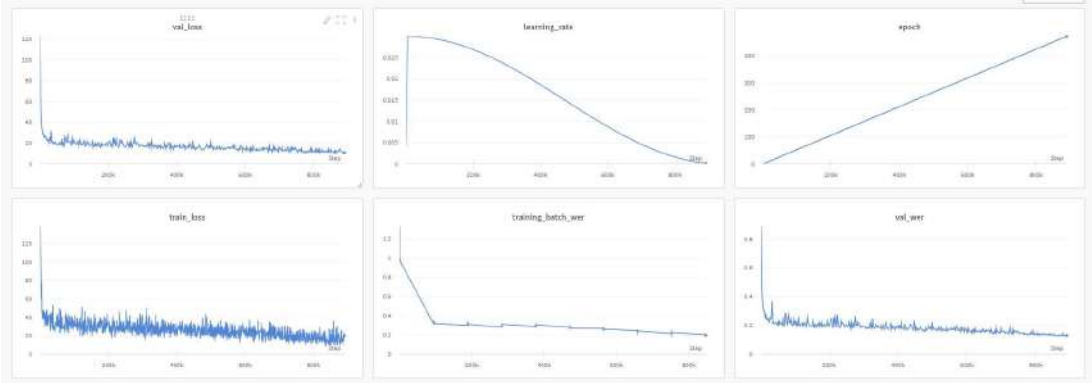
Achievements:

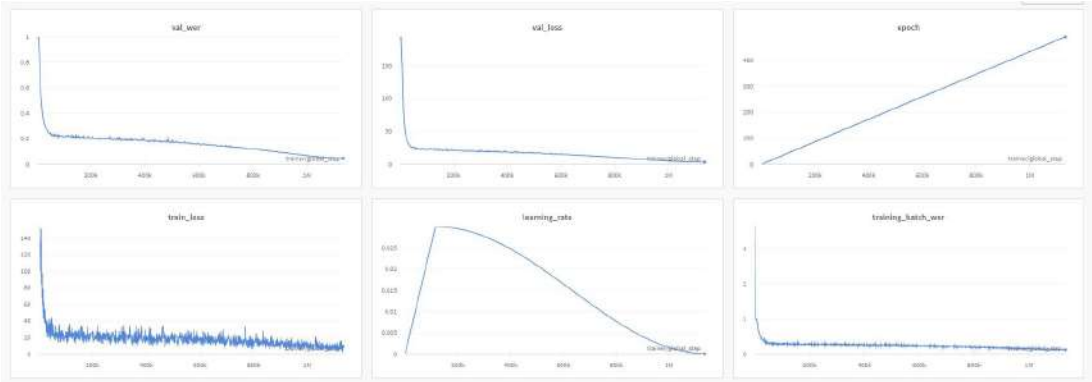
1. Winner for English ASR Challenge organized by IITM
2. Performed single and multi-node ASR training on PARAM Siddhi AI compute node
3. Deployment of RIVA End-to-End ASR pipeline on PARAM Siddhi Inference node
4. Designed and Developed Speech Technology Suite
5. Online and Offline Multilingual STT system for Hindi, Marathi and English languages
6. PoC for AI enabled Automatic subtitle framework
7. PoC for Speech-to-Speech Conversational AI system
8. PoC for Gender and Spoken Language Identification

Experimental Results:
Training and Inferencing on PARAM Siddhi AI

Table : Result

S.No.	Language	Speech Corpus (Hrs.)	Training Time (Hrs.)	Accuracy (%)	ASR Inference Time
1	Hindi	2600	72:00	95	1Hrs. data in 10Min.
2	English	2500	70:00	97	1Hrs. data in 10Min.
3	Marathi	1000	30:00	88	1Hrs. data in 10Min.





Benefits & experience of using NPSF:

1. With the help of PARAM Siddhi-AI system, we are able to build and benchmark ASR models on large speech data
2. It not only allows us to build the model but also it speed up the training and optimized the inference time too
3. Deployed ASR service at PARAM Siddhi-AI Inference node using kubernetes
4. Performed various experiments for ASR building approaches on fast and efficient way

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work :

1. It would be great help if we can have a dedicated compute node
2. Right now the data across multiple users under the same project is not accessible if that is resolved the data duplicity can be reduced to great extend

Title of the work carried out: R&D on building DNN based speech recognition system under National Supercomputing Mission (NSM)

Name & Designation of the Chief Investigator: Ajai Kumar, Senior Director, AAIG & GIST, C-DAC Pune.

E-mail Id: ajai@cdac.in

Institution Name: C-DAC Pune

Application Domain: Conversational AI

Research Challenge/s: N/A

Work carried, Milestone, Achievements & Graphs, Plots: N/A

Benefits & experience of using NPSF: N/A

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : N/A

Title of the work carried out: Development of HPC centric real-space numerical methodologies towards exa-scale architectures for large-scale ab-initio modeling of materials

Name & Designation of the Chief Investigator: Dr. Phani Sudheer Motamarri, Assistant Professor

E-mail Id: phanim@iisc.ac.in

Institution Name: Indian Institute of Science, Bangalore

Application Domain: Computational Materials Physics

Research Challenge/s: During the preview access, we installed our in-house DFT-FE code and the installation took lot of time as we had difficulties installing required dependencies. After successful installation, we had initial difficulty in getting our in-house GPU code (DFT-FE) scalable across multi-GPU nodes. The rail on which the code was running was not connected with infiniband. This got eventually rectified and then later we observed good scalability up to 40 GPUs (5 Nodes) as we were able to run only on 5 nodes in the preview access. After the project access in Dec 2021, we again installed our code and could not run beyond 1 node as there was heavy queuing time since max run wall time of each job is 7 days. There were several jobs which were running for more than 5 days, and we could not finish scaling study.

Work carried, Milestone, Achievements & Graphs, Plots:

I am one of the principal developers of our in-house massively parallel hybrid CPU-GPU DFTFE code, a quantum modeling software using Density Functional Theory. This code was ACM Gordon Bell Finalist in 2019. In the preview access period, we were trying to study the scalability aspects of the DFT-FE code on PARAM Siddhi. We took a problem with 1.72 million degrees of freedom and performed a scalability study starting from 8 GPUs, 16 GPUs, 24 GPUs, 32 GPUs and 40 GPUs. The percentage scaling efficiency relative to 8 GPU run was 90%, 78%, 70% and 62% on 16 GPUs, 24 GPUs, 32 GPUs and 40 GPUs respectively.

Benefits & experience of using NPSF: We took a problem with 1.72 million degrees of freedom and performed a scalability study starting from 8 GPUs, 16 GPUs, 24 GPUs, 32 GPUs and 40 GPUs. The percentage scaling efficiency relative to 8 GPU run was 90%, 78%, 70% and 62% on 16 GPUs, 24 GPUs, 32 GPUs and 40 GPUs respectively. We hope access to large number of GPUs through the recent project access will enable large-scale quantum modeling of materials and thereby address complex material science problems.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Siddhi-AI for your research work : Max walltime of around 7 days for any job will result in huge waiting times which is not beneficial for efficient use of the cluster by all users.

7.2 Appendix 'B' PARAM Yuva-II Work Reports

Work Report 1 Summary

Title of the work carried out: DFT based Study of Topological Insulators for Spintronics Application and organic-inorganic perovskite for Optoelectronics

Name & Designation of the Chief Investigator: Dr. Ramesh Kumar, Assistant Professor, Dept. of Physics, GJU S & T, Hisar-125001

E-mail Id: ramesh85@gjust.org

Institution Name: Guru Jambheshwar University of Science and Technology, Hisar-125001, Haryana (INDIA)

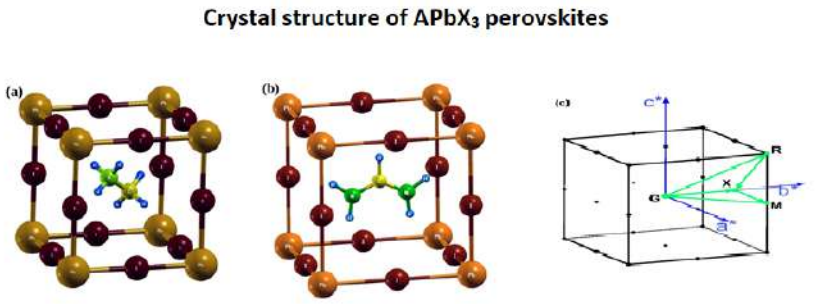
Application Domain: Computational Physics, Structural Engineering and Material Science

Research Challenge/s: Sometimes, calculations go into waiting list.

Work carried, Milestone, Achievements & Graphs, Plots:

Structural and Electronic Properties of Perovskites Materials

The organic-inorganic hybrid compounds APbX3 (A= CH3NH3+ (MA), CH (NH2)2+ (FA) and X = Cl, Br and I) with a perovskite structure are of particular interest due to their potential applications in highly efficient solar systems.In this work, we studied the structural and electronic properties of APbX3 (A= CH3NH3+ (MA), CH (NH2)2+ (FA) and X = Cl, Br and I) perovskites using DFT methodology implanted in Quantum Espresso code.

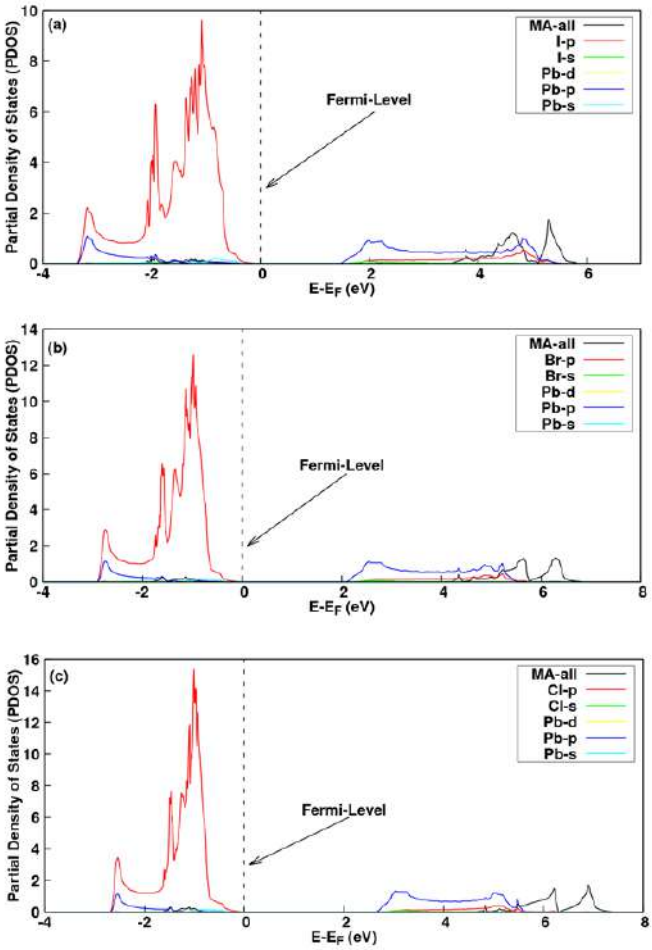


(a) Cubic Crystal structure of $MAPbI_3$ (b) Cubic Crystal structure of $FAPbI_3$ (c) represents the corresponding first Brillouin zone with high symmetric k-points

The substitution of the Br and Cl atoms in place of I atoms to compute the lattice constants for MAPbBr3 and MAPbCl3 perovskites. The calculated lattice constants for these perovskites are 6.23 Å and 6.07 Å, respectively, which are in good agreement with the experimental results.

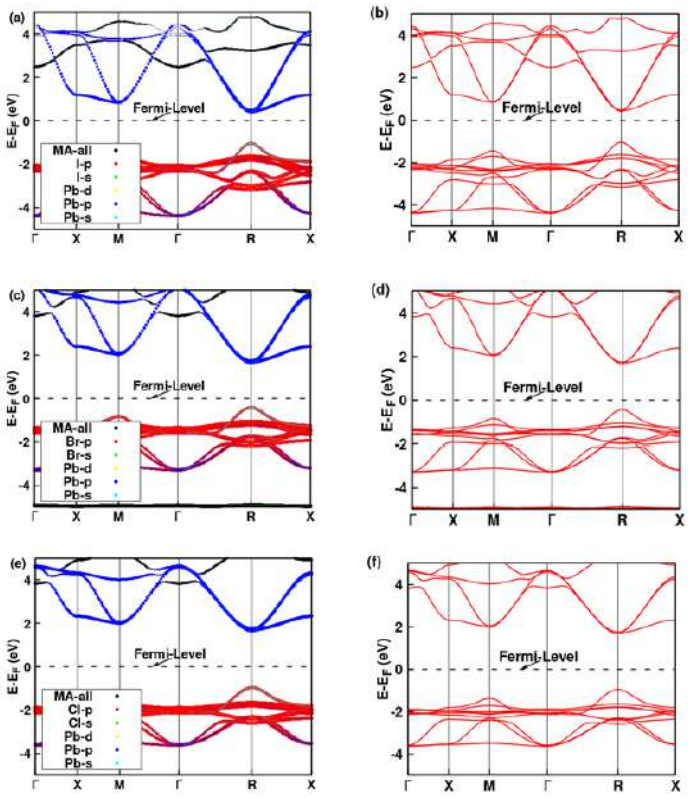
Electronic Properties

To investigate the electronic properties of APbX3 perovskites, the density of states and electronic bulk band structure for these compounds are computed.



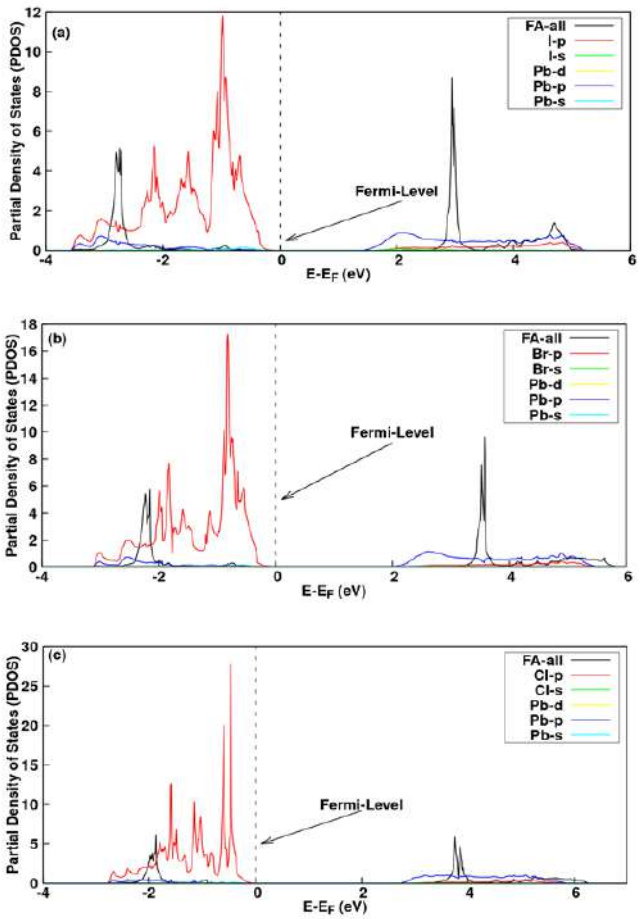
Partial density of states (PDOS) for perovskites (a) $MAPbI_3$ (b) $MAPbBr_3$ and (c) $MAPbCl_3$

The calculated value of the bandgap for MAPbI3 is 1.45 eV. Further, the replacement of the I atoms with Br atoms then the CBM shifts upward thus increasing the bandgap up to 2.1 eV. Similarly, in the case of MAPbCl3, the value of the bandgap is found to be 2.60 eV.



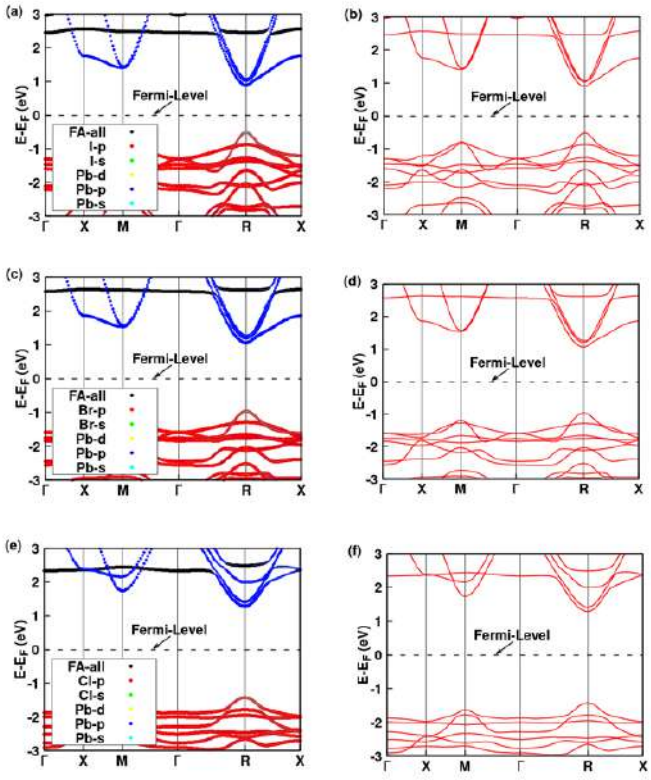
(a-b) The orbital projected bulk band structure and electronic bulk band structure of $FAPbI_3$, (c-d) $FAPbBr_3$ and (e-f) $FAPbCl_3$ perovskites respectively

Now the electronic properties of FAPbX3 perovskites are discussed.



Partial density of states (PDOS) for perovskites (a) $FAPbI_3$ (b) $FAPbBr_3$ and (c) $FAPbCl_3$

The calculated value of the bandgap for FAPbI3 is 1.41 eV. Further, the substitution of the I atoms with Br atoms shift the CBM, a little upward and VBM shift downwards thus increasing the bandgap up to 2.02 eV. Similarly, in the case of FAPbCl3, the value of the bandgap is found to be 2.70 eV.



(a-b) The orbital projected bulk band structure and electronic bulk band structure of $FAPbI_3$, (c-d) $FAPbBr_3$ and (e-f) $FAPbCl_3$ perovskites respectively

Finally, the Van der Waals (vdW) interactions are included to check the effect of these interactions on the lattice parameter and energy bandgap of APbX3 compounds. Grimme-D2 method is used to calculate the optimized lattice parameter and then fully relax the structure to obtain the ground state energy. The results obtained for all compounds of configurations APbX3 are tabulated in Table 1 as shown below.

Table 1 : Result

Compound	vdW-DF		Grimme-D2	
	Lattice Parameter	Bandgap	Lattice Parameter	Bandgap
	(Å)	(eV)	(Å)	(eV)
MAPbI3	6.47	1.7	6.37	1.42
MAPbBr3	6.22	2.23	6.14	1.98
MAPbCl3	6.01	2.75	5.94	2.55
FAPbI3	6.48	1.61	6.39	1.39
FAPbBr3	6.25	2.1	6.18	1.94
FAPbCl3	6.15	2.78	6.10	2.63

Conclusion: The structural and electronic properties of APbX3 perovskites are studied by replacing A with methyl ammonium CH3NH3+ (MA) and formamidinium CH(NH2)2+ (FA) and X with Cl, Br, and I using density functional theory calculations in Quantum Espresso Code. These compounds are found to be stable in a cubic structure having space group Pm-3m. The value of the lattice parameter increased from 6.07 Å to 6.39 Å by substituting halide atoms in

the order of Cl, Br, and I, and the corresponding bandgap decreased from 2.60 eV to 1.45 eV in MAPbX3. Similarly, by substituting halide atoms in the order of Cl, Br, and I, the lattice parameter increased from 6.20 to 6.41, and the corresponding bandgap decreased from 2.70 eV to 1.41 eV in FAPbX3 compounds. Further, the effect of Van der Waals interactions is investigated on the lattice parameters as well as the energy bandgap of these perovskites.

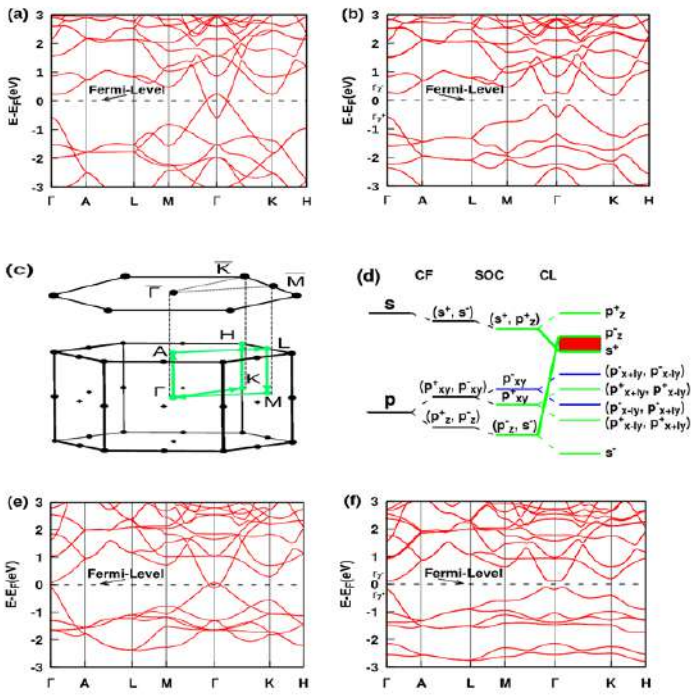
Future Work: Now we are working for calculating the optical properties of perovskite material for their possible application in perovskite solar cells.

This work is under process and will be communicated very soon in reputed journal for publication: We have carried out the calculations on NPSF PARAM Yuva-II system to get the structural, electronic and topological properties of KBaBi and NaCaBi compound. This work has been published in the international journal named "Journal of Physics and Chemistry of Solids" under the title "Structural, electronic and topological properties of NaCaBi and KBaBi compounds"

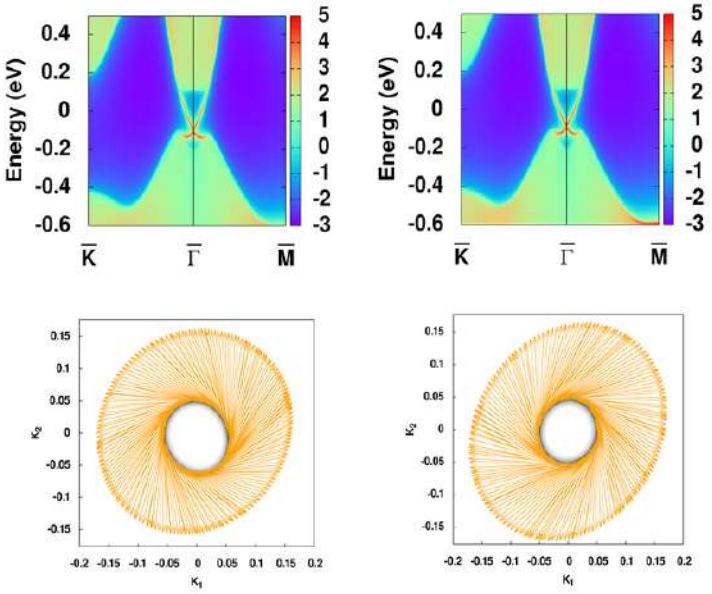
Citation Details : "Sanjeev et al. Structural, electronic and topological properties of NaCaBi and KBaBi compounds. Journal of Physics and Chemistry of Solids 161 (2022) 110416.

In this work we had investigated the structural, electronic and topological properties of NaCaBi and KBaBi compounds without and with spin-orbit coupling effect by employing density functional theory in Quantum Espresso code. Without spin-orbit coupling, NaCaBi and KBaBi compounds behave as a type-I nodal line semimetal and form a nodal loop around the Γ-point in the k z = 0 plane of Brillouin zone. When the bulk states were projected onto the (001) surface, a drumhead-like surface state was reported inside the nodal line for both compounds. The s/p band inversion in NaCaBi and KBaBi compounds were reported due to the strong spin-orbit coupling with band inversion energy of 0.87 eV and 0.32 eV respectively. The spin-orbit coupling in NaCaBi and KBaBi compounds induced the band gap of value 0.32 eV and 0.21 eV respectively. Z2 indices for NaCaBi and KBaBi are found (1; 000) which indicates that NaCaBi and KBaBi are strong topological insulators. The topological surface states and corresponding spin-texture were also calculated for both compounds which show a single Dirac cone at Γ-point with Dirac point lying below the Fermi-level.

Some of the important figures are given below:



The bulk electronic band structure of NaCaBi (a) without and (b) with SOC. High symmetric k-point path in the BZ of hexagonal structure and its projection onto the (001) surface (c). (d) Schematic diagram to represent the band inversion between the s and p orbitals of Bi at Γ -point. The effect of crystal field splitting (CF), SOC and coupling between Ca (Ba) – Bi layers (CL) on the VB and CB around the Fermi-level at Γ -point. The bulk band structure of KBaBi (e) without and (f) with SOC.



Surface states (SS) and corresponding spin texture around the Fermi-level for (a), (c) top surface and (b), (d) bottom surface of KBaBi.

Highlights Of Work:

1. The NaCaBi (KBaBi) compounds have crystallized in hexagonal crystal structure with optimized lattice parameters a = b = 5.5507 (6.1599) and c =6.7938 (7.5680) respectively.
2. Without SOC, we reported that NaCaBi and KBaBi behave like a type-I NLSM with a nodal loop and drumhead-like nodal surface around the point protected by the mirror symmetry in the kz = 0 plane.
3. The electronic structure for NaCaBi (KBaBi) compounds under the influence of SOC, showed the s/p band inversion with band gap 0.33 eV (0.21eV) and corresponding band inversion energy 0.87 eV (0.32 eV) respectively.
4. The calculated topological properties for NaCaBi (KBaBi) compounds suggested that these systems are strong topological insulators with Z2 indices of (1;000).
5. The surface Dirac cone of NaCaBi (KBaBi) compounds is found to have a right-handed spin texture for the bottom surface state whereas left-handed spin texture for the top surface states of the slab.
6. The calculated value of bulk band gap 0.31 eV for NaCaBi provides a high potential for room-temperature spintronics devices

Societal impact of work:
These are wide gap topological insulators which are beneficial for supercomputing and spintronics. TIs are also used as a good thermoelectric material.

Future Work: Now we are working on to investigate the structural, electronic and

topological properties of Sr3Bi2 and Ca3Bi2 compounds.Thermoelectric Performance of PtX2 (X= Se, Te) Monolayers

In this work, we have investigated the structural, electronic, and thermoelectric properties of PtX2 (X= Se, Te) monolayers using ab-initio calculations in conjunction with semi-classical Boltzmann transport theory. Phonon dispersion curves have been investigated using the PHONOPY package Figure 1. The electronic transport properties of PtX2 monolayers are studied using semi-classical Boltzmann transport theory as implanted in the BoltzTraP code. For these properties, the electronic structure is computed by dense k-point mesh of size 60×60×1 for Brillouin zone sampling. The BoltzTraP code calculated the electrical conductivity ($\sigma\ \tau$), Seebeck coefficient (S), electronic thermal conductivity (Ke/τ) in terms of τ. Now the τ is used to calculate the exact electrical conductivity (σ) and electronic thermal conductivity (Ke). The lattice thermal conductivity (K1) is obtained by linearized phonon Boltzmann equation by employing the phono3py code.

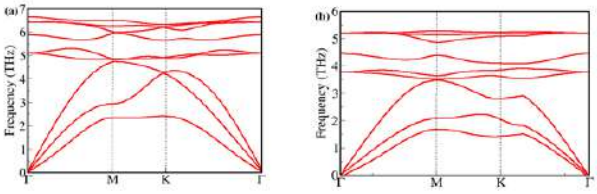


Figure 1: Phonon dispersion curve for monolayer (a) $PtSe_2$ and (b) $PtTe_2$, respectively

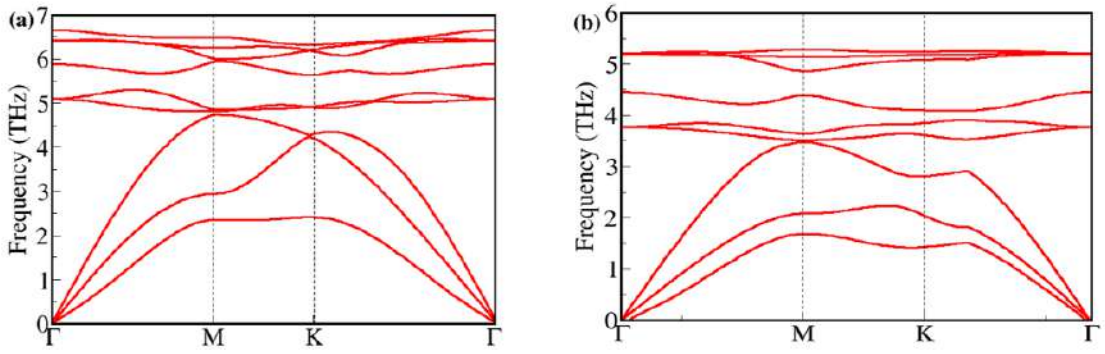


Figure 1: Phonon dispersion curve for monolayer (a) $PtSe_2$ and (b) $PtTe_2$, respectively.

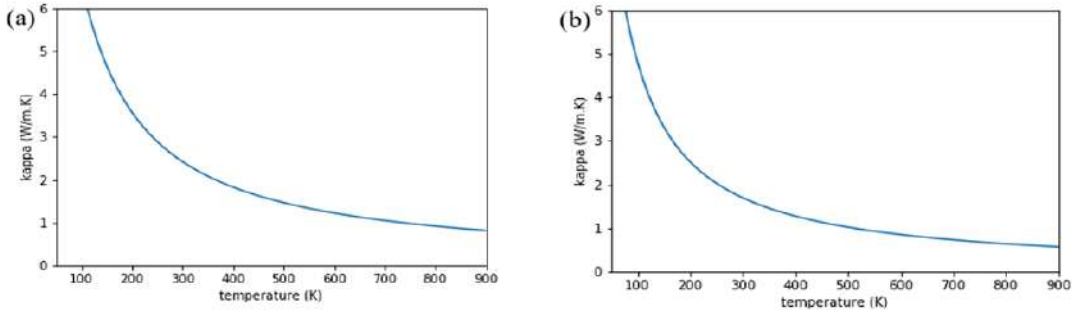


Figure 2: Lattice thermal conductivity (κl) for monolayer (a) $PtSe_2$ and (b) $PtTe_2$, respectively.

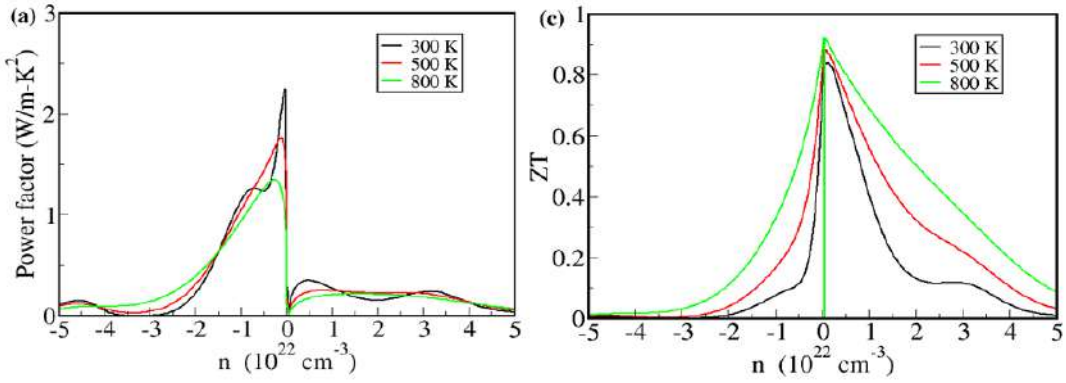


Figure 3: Calculated (a) & (b) power factor ($S^2\sigma$) and (c) & (d) figure of merit (ZT) as a function of carrier concentration (n) corresponding to monolayer $PtSe_2$ and $PtTe_2$.

This work is under process and will be communicated very soon in reputed journal for publication.

Future Work: Now we are working on to investigate the structural, electronic and thermoelectric properties of layers of CrSe2 compound.

All above mentioned properties requires a heavy computational facility. High dense k-point calculation is only possible with nearly 80 processor which can be done only by NPSF PARAM Yuva-II system. In Phonopy and Phono3py, a large number of supercells has been created and takes a lot of time nearly 15-20 days with 100 processors. We have acknowledged NPSF PARAM Yuva-II system in our above-mentioned work which is under review, not published up to now. All these types of calculations are not possible to run without NPSF PARAM Yuva-II system. Therefore, our team is highly thankful for this computational support.

Benefits & experience of using NPSF:

This platform enables us to do calculations quickly and efficiently. The storage space was adequate for all sorts of calculations, which saved our time from regularly backup the data from server. The most significant benefit is that it is free for needy students who would otherwise struggle to afford a premium account. This facility is proved to be milestone for theoretical researchers.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work :

I would like to thank NPSF PARAM Yuva-II to providing me opportunity to work on this platform. This supercomputing facility saved my time by doing fast calculations and providing the storage space for data at free of cost. Without NPSF PARAM Yuva-II computational support, we can't imagine this type of calculations. Thanks to whole CDAC team for providing this high-end computational facility to us.

Title of the work carried out: Structure and Properties of Novel Transition Metal Dichalcogenide Nanosheets

Name & Designation of the Chief Investigator: Dr. T. J. Dhilip Kumar, Associate Professor, Department of Chemistry, IIT Ropar

E-mail Id: dhilip@iitrpr.ac.in

Institution Name: Department of Chemistry, IIT Ropar

Application Domain: Material Sciences

Research Challenge/s: The waiting time to start the calculation is very long running into days to week. If there is any mistake in the input file, then again to resubmit the job, one has to wait for long time.

Work carried, Milestone, Achievements & Graphs, Plots:

Tuning Structure, and Electronic Properties of Non-Metal Atom Doped Janus TMD s for Hydrogen Evolution Reaction

The doping of hetero-non-metal atoms into the conventional Transition Metal Dichalcogenide (TMD) monolayer sheets is reported to tune their structural, electronic, magnetic, and catalytic properties. Herein, the physicochemical properties of Janus MoSSe monolayer with the doping of atoms viz. B, C, N, and P are systematically studied using density functional theory. The high binding energies for the doping of non-metal atoms into TMD sheets show energetic stability of the doped Janus sheets. The doping reduces the band gaps as compared to pristine sheet because of the introduction of the bands near the Fermi region. The doping of nonmetal atoms also tunes the magnetic properties of Janus nanosheets and broaden up their applications in spintronics. The catalytic activity of the Janus TMDs for Hydrogen Evolution Reaction (HER) is explored which possess inherent strain due to asymmetry. The density functional theoretical studies of the pristine and non-metal atom doped Janus TMDs as HER catalysts are reported in terms of Gibbs free energy which depends on the electronegativity of dopants. Overall results indicate that the boron doped Janus sheet possesses reduced band gap and tunable work function which contributes to the superior catalytic performance for HER even in the absence of external strains and large basal plane vacancies.

the Perdew-Burke-Ernzerhof (PBE) form of the generalized gradient approximation (GGA) for the exchange-correlation functional. The Grimme-D3 exchange-correlation function was used for the correct consideration of chemisorption and long range interactions. A 4x4x1 super-cell of MoSSe was considered as a model nanosheet for the adsorption of hydrogen. A cut-off energy of 450 eV was chosen for 3 plane-wave basis set. The unit cell of MoSSe nanosheet was relaxed with τ-centered Monkhorst-Pack K-point mesh of 5x5x1 in the first Brillouin zone. The energy convergence limit was kept to be 10^{-8} eV . The ionic positions were relaxed till the magnitude of

the force on each ion in the cell becomes less than 10^{-3} eV/Å. In order to avoid the interations between the adjacent layers, a vacuum of 15 Å was introduced in z-direction for all the calculations. Furthermore, the effect of non-metal atom doping on the charge transfer properties was also computed by performing Bader charge analysis.

Structures and Stabilities:
A relaxed geometry of pristine MoSSe 4x4x1 supercell is shown in Figure 1 ((a) top view and (b) side view). The Janus transition metal dichalcogenide sheets are three layered structure where the transition metal atom M (Mo) layer is sandwiched between the different chalcogen atom layers (X=S and Y=Se). The stability of the pristine sheets have been computed in terms of phonon band dispersion band structures. The phonon band dispersion band structure for pristine MoSSe sheet is shown in Figure 2. The absence of negative vibrational frequencies indicate that the sheet is thermodynamically stable. The formation energies for Mo, S, and Se defected sheets are obtained are found to be -6.04, -4.09, and -3.85 eV, respectively. The formation energies are found to be less negative for the S/Se defected TMD nanosheets indicating that the non-metal atom defected sheets are more stable than that of metal defected sheets. This also supports that the doping of foreign atoms at non-metal atom sites is energetically more feasible than that of metal doping.

The doping of non-metal atoms in the TMD sheets is considered as a two step process i.e. the vacancy creation followed by the doping of the foreign atoms at the vacant S/Se sites. It is observed that the doping of B, C, N, and P atoms at the Sulfur or Selenium defects results in the slight structural changes in the Janus monolayers which is obvious due to the difference between the atomic sizes of the dopants and the S/Se atoms. That is the reason why, the doping of B, C, and N atoms at the defected sites in the MoSSe monolayers are observed to form a concave surface around the dopants as their atomic radii is smaller than that of S/Se atom. The bond lengths between B-, C-, N-, or P- and Mo are reported in Table 1 from which it can be seen that the bond lengths between the dopant and the transition metal atoms are shortened than that of S/Se-Mo.

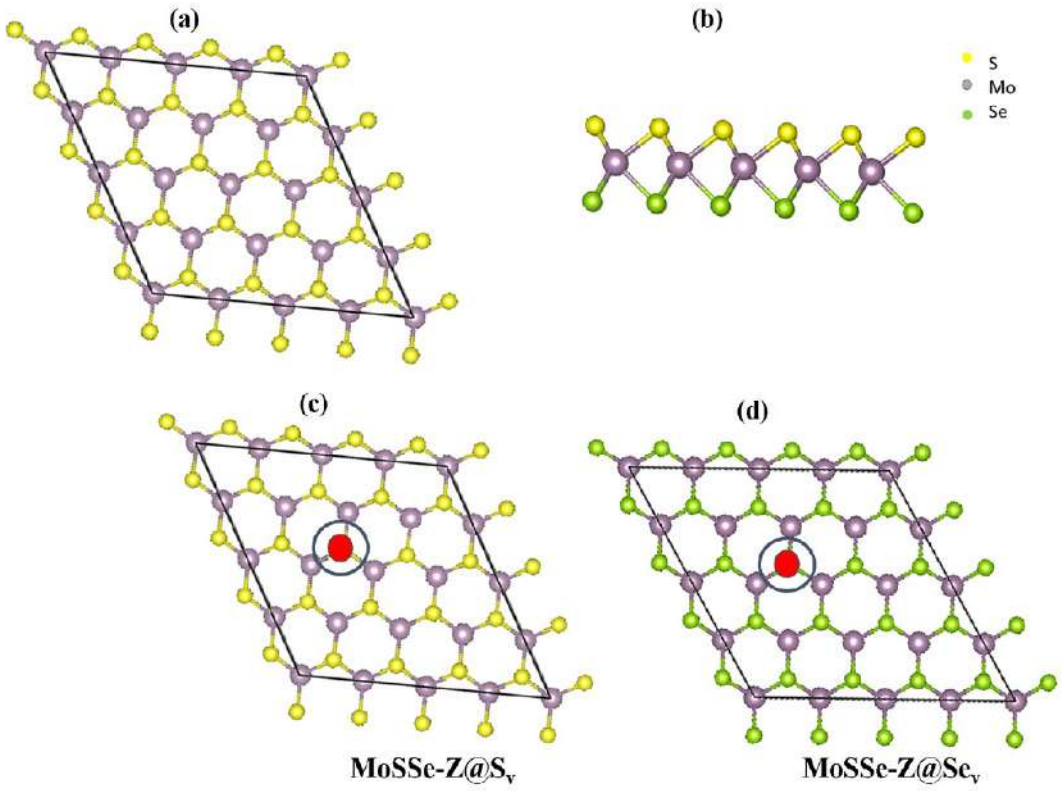


Figure 7.1: Pictorial representations of pristine MoSSe Janus sheet: (a) top view (b) the side view (c) MoSSe-Z@Sv and (d) MoSSe-Z@Sev nanosheets, where Z= B, C, N and P at the S and Se vacant sites, respectively.

Table 1: Bond distances between Mo and non-metal atoms in MXY − Z@X_v and MXY − Z@Y_v nanosheets in Å.

System	*Bond length*					
	S	Se	B	C	N	P
MoSSe − Z@S_v	2.424	2.542	2.134	2.037	2.018	2.429
MoSSe − Z@Se_v	2.424	2.542	2.112	2.021	2.015	2.415

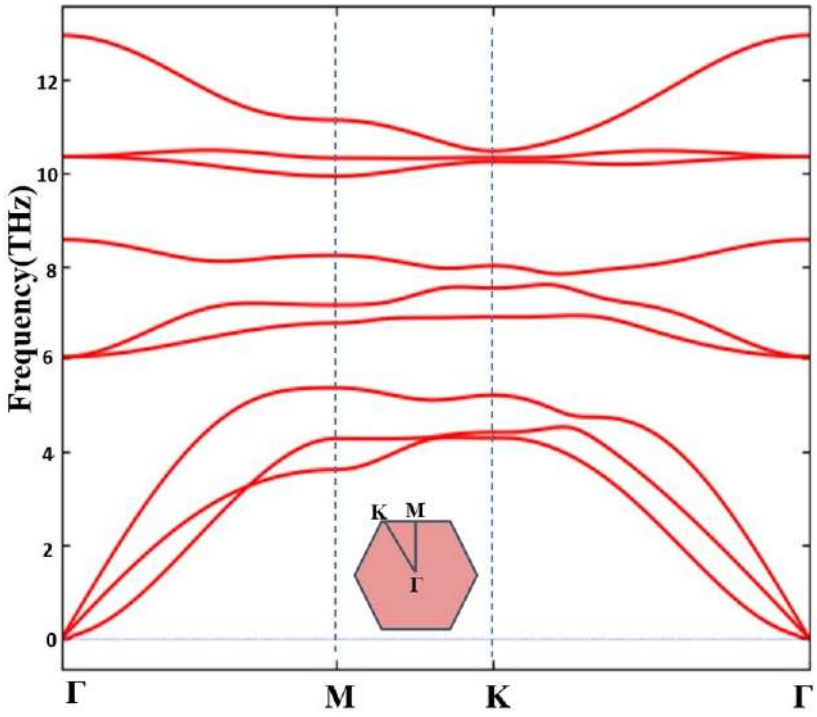


Figure 7.2: The phonon dispersion band structure of pristine MoSSe.

Table 2: Binding energies in (eV), fermi energies (eV), work function (eV) and magnetic moments (μB) of non-metal (boron, carbon, nitrogen, and phosphorus) atom doped at S and Se vacancy in MXY − Z@X_v and MXY − Z@$Y_v$nanosheets.

System	***Binding Energy***				***Fermi Energy***				***Work Function***				***Magnetic Moment***			
	B	C	N	P	B	C	N	P	B	C	N	P	B	C	N	P
MoSSe − Z@S_v	-5.46	-7.13	-6.10	-4.63	0.89	0.76	0.76	0.93	5.57	5.49	5.46	5.55	0.99	0.00	0.99	0.99
MoSSe − Z@Se_v	-5.39	-7.09	-6.06	-4.56	1.05	0.90	0.86	0.86	5.62	5.58	5.53	5.60	0.92	0.00	0.99	0.94

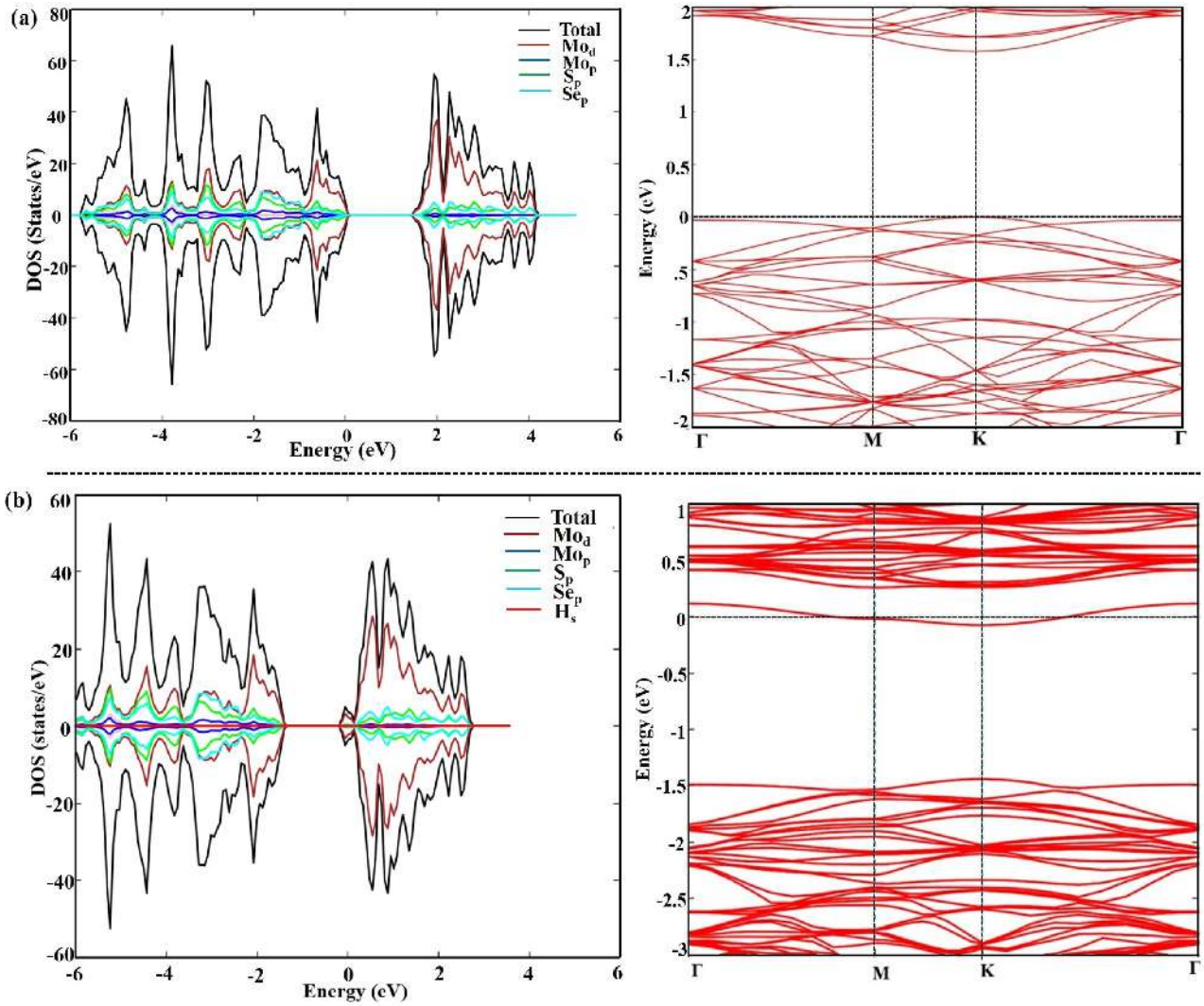


Figure 7.3: The total density of states (DOS), projected density of states (PDOS), and band structures of (a) pristine MoSSe and (b) MoSSe + Hads nanosheets.

Whereas, the doping of P atom at the sulfur vacancy forms a convex surface around the surface because of the slightly larger atomic size of P compared to S. That is why the bond-length of Mo-P is obtained to be slightly longer than that of the Mo-S. Futhermore, the stability of the non-metal atom doped Janus monolayers was computed in terms of binding energy. The values of binding energies for the doping of non-metal atoms at S and Se vacancies in MoSSe nanosheets are tabulated in Table 2. The negative values indicate that the doping of these non-metal atoms is an energetically feasible process. The binding energy is found to be comparatively lower for the phosphorus doping in all the cases. Whereas, it is observed to be more negative for carbon and nitrogen doping indicating that the binding strengths are higher for these non-metal atoms. The structural changes may also impact the electronic properties which are discussed below.

Electronic Properties:

The effect of the doping of B, C, N, and P atoms on the electronic properties of Janus TMD nanosheets is studied. The spin-polarized band structures, density of states (DOS), and projected density of states (PDOS) of pristine MoSSe nanosheets are computed and shown in Figure 3. The direct band gaps of 1.57 eV is observed for pristine MoSSe nanosheet. The mirror symmetry in both the spin states indicates the non-magnetic semiconducting nature of pristine MoSSe sheet (Figure 3). The band gap value of MoSSe nanosheet is also observed to be in excellent

agreement with the reported literature results. The computed PDOS of pristine sheets show that both valence as well as conduction bands are majorly dominated by d-orbitals of transition metal atoms i.e. Mo, whereas the deeper regions consist of s- and porbitals of S and Se atoms and is responsible for the covalent bonding interactions in the Janus TMD sheets.

The doping of non-metal atoms at the S and Se vacancy sites are found to introduce impurity levels in sheets close to the Fermi energy region as shown in Figure 3. An introduction of impurity bands near the Fermi region is responsible for the decrease of band gap values than that of the respective non-defected sheet. For example, in the case of boron doped sheets, the bands are appeared above the valence band, whereas carbon doping results in the band formation just below the conduction band.

The effect of non-metal doping on the magnetic properties of Janus TMD 8 nanosheets is also computed in this work which indicates that the boron-, nitrogen-, and phosphorus doped at the Sulfur or Selenium vacancies in the MoSSe nanosheets show the magnetic moment of approximately . 1μB.The magnetic moment occurs due to the presence of unpaired electrons. For example, for the boron-doped sheets, unpaired electrons locate at the boron p-orbitals and the adjacent metal d-orbitals. However, the carbon-doped nanosheets are observed to be non-magnetic due to the absence of unpaired electrons.

The work function values also varies with the increase or decrease in the number of density of states near the Fermi level. The work function value for pristine Janus sheet obtained is found to be 5.67 eV. It can be seen from Table 2 that the work function values for the non-metal atom doped monolayers are slightly lower than that of pristine sheet. Along with that, work function in the doped sheets varies with the dopant indicating the possibility to tune the properties of such sheets in various applications such as gas sensors, electrocatalysis, etc.

The charge transfer due to the doping of non-metal atoms was also calculated by performing Bader charge analysis in the present work. The Bader charge analysis shows that the doped atoms attain negative charges. The boron, carbon, nitrogen, and phosphorus atoms gain 0.31, 0.76, 0.95, and 0.35 electron from the sheet due to their high electronegativity.

The above mentioned results indicate that the electronic as well as magnetic properties of Janus TMD monolayer sheets can be tuned by doping different nonmetal atoms which implies its applications in various fields such as batteries, sensors, catalysis, etc.

Benefits & experience of using NPSF:

NPSF Param Yuva-II facility is an add on system. Whenever our in-house small cluster system is overloaded, we make use of Param Yuva-II facility.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work :

Please reduce the waiting time. To maximize the output, the submit job should run within 8 hours of submission.

Work Report 3 Summary

Title of the work carried out: Geospatial Information Extraction from Big Satellite Data

Name & Designation of the Chief Investigator: Dr. Sivakumar V, Joint Director

E-mail Id: vsivakumar@cdac.in

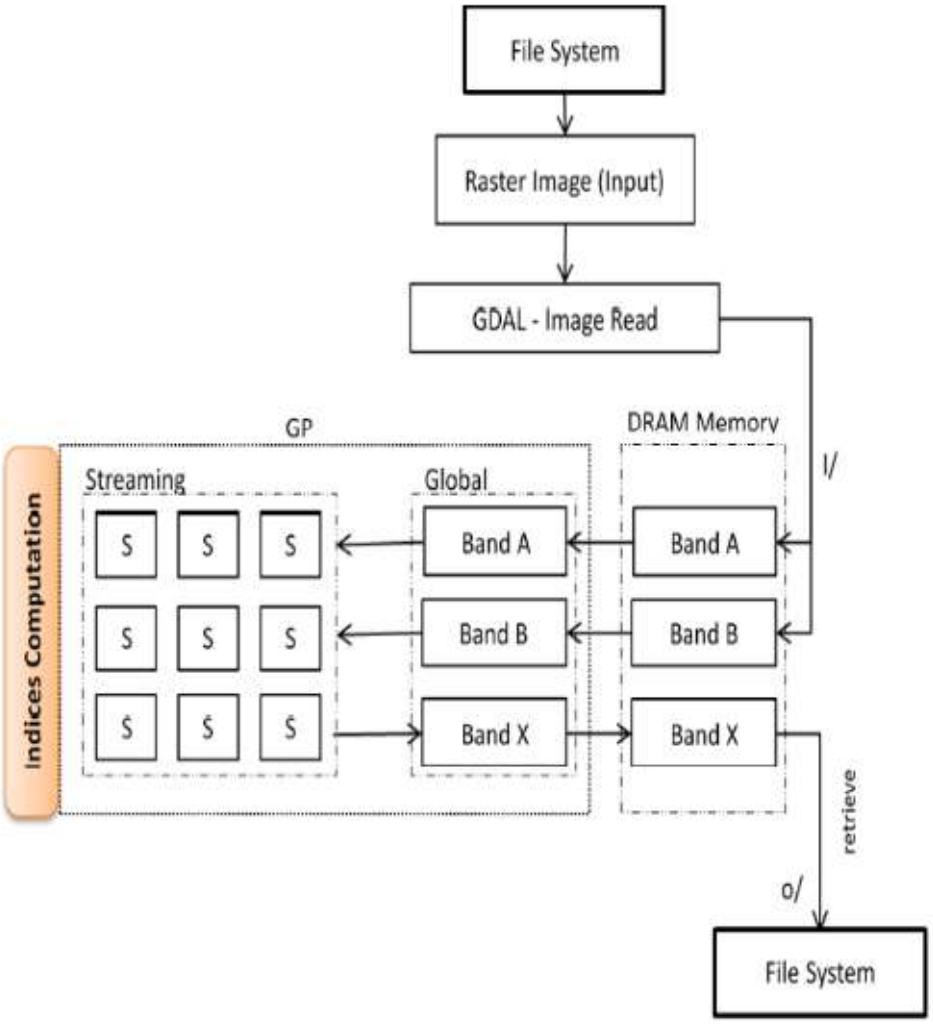
Institution Name:ESEG Group, C-DAC, Pune

Application Domain: Geo-Inforamtics

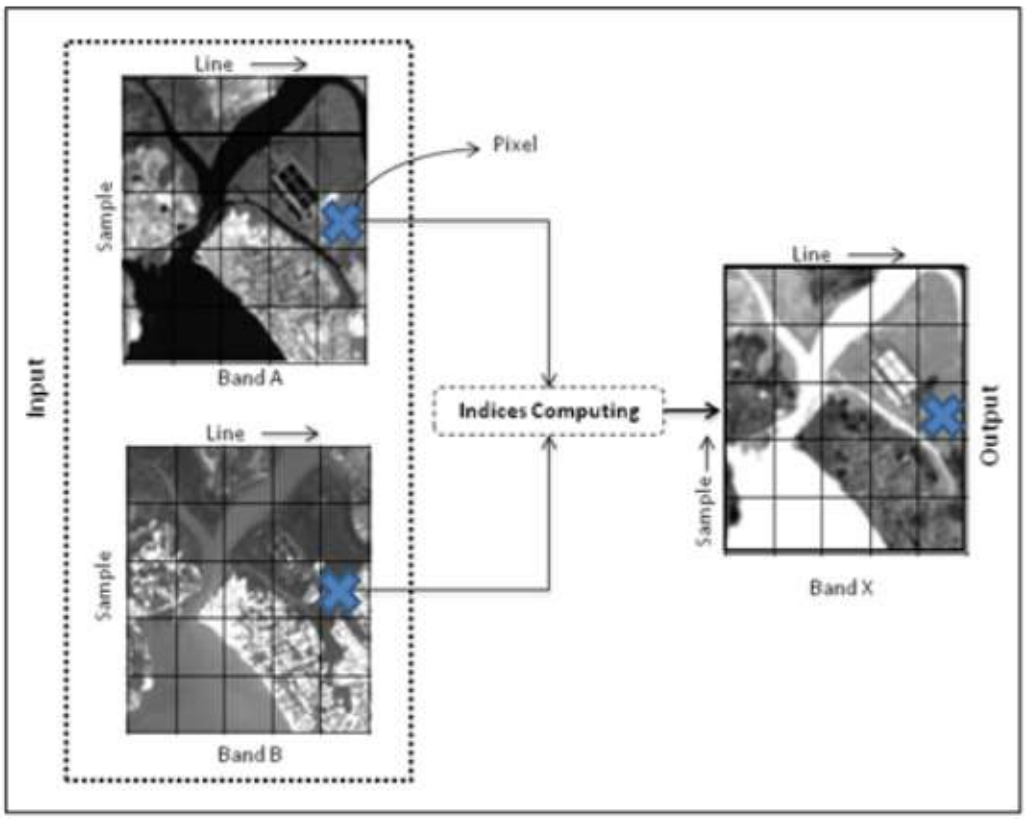
Research Challenge/s: Satellite images are important sources for extracting geographic information and analysing it using various methods such as NDVI, MNDWI, SAVI, classification, etc. to extract landscape elements. Earth observational satellite data size and volume are rapidly increasing due to enhancement of the spatial, spectral, temporal and radiometric resolution of the satellite sensors. Remote sensing data are big data due to their volume, variety and velocity. These big data emerged as a new paradigm to provide unprecedented data content and value for Digital Earth. However, data processing technology poses main challenges, especially related to computing speed and efficiency in handling the large volume of satellite data in real time. Relatively low-cost high-end processors are conventionally used for satellite data analysis, though these systems are not sufficient to process very large images. Therefore, it is agreed that conventional approaches are inadequate for these new generation sensors.

Work carried, Milestone, Achievements & Graphs, Plots:

Landsat-8 Operational Land Imager (OLI) imagery from the USGS data archive database was used for demonstrating the present study. The image area covers the North Mumbai area. April month (12 April, 2014) data (cloud free) have been utilised for the experiment. Below flow diagram (Figure 1) shows a detailed processing flow adopted in this study. Algorithms were implemented in C using CUDA due to its advantages over other GPU APIs. CUDA is a general-purpose parallel architecture, with a programming model and software environment that allows developers to use CUDA, a high-level programming language, in applications with fine-grained parallelism and execute them in massive parallel threads. Stacked satellite imagery was uploaded to the file system and desired bands (b3, b4, b5 & b6) were read and transferred to DRAM (Dynamic random-access memory) of NVIDIA M2090 GPU using GDAL open-source library. The execution was parallelized using C-DAC's PARAM Yuva-II supercomputer, by assigning one thread per pixel (Figure 2). The computation of output for one pixel in the target image is independent of computing other pixels. We enable one thread to compute one pixel of the original image with CUDA. In the procedure, the grid is divided into blocks and each block is composed of threads. Then each thread can be executed independently to compute the relevant pixel of the target image. We also executed the MNDWI and SAVI algorithms over serial computation approach.



Algorithm implementation and satellite data processing flow



Parallelization methods for indices computation from satellite imagery

Benefits & experience of using NPSF:

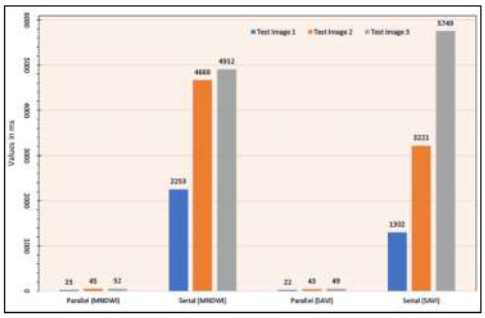
Two different types of indices computations techniques have been tested on NVIDIA CUDA-enabled GPU which is embedded with C-DAC's PARAM Yuva-II supercomputer. A GPU is used for these experiments and it is the NVIDIA™ Tesla M2090, it features 512 processor cores operating at 1.3 GHz, with peak double precision floating point performance of 665 GFlops, Peak single precision floating point performance of 1331 GFlops, total dedicated memory of 6 GB, 1.85 GHz memory (with 384-bit GDDR5 interface) and memory bandwidth of 177GB/s. We implemented MNDWI and SAVI algorithms on GPU parallel and serial approaches for 3 sets of satellite data. The MNDWI and SAVI indices are computed from Landsat 8 OLI satellite imagery. We implemented the spatial distribution of MNDWI and SAVI are shown in Figure 6. The minimum MNDWI and SAVI values of the ground surface are around 0.17, 0.46 and maximum values are around 0.325, 0.81 respectively. The execution time with the total number of pixels in an image is compared to validate the performance. Remote sensing–based spectral indices provide an efficient method in the automated identification of land use and cover classes. In the obtained results it is evident that indices calculation over satellite imagery gave promising results with rapid speed. The results show that big data can be handled much easier with GPU parallel computing model. This technique would be more relevant in handling big satellite data with very large aerial coverage in applications like natural resource monitoring and estimation, urban development, disaster management and agriculture. This result indicates that the execution time depends on the algorithm. Figure 4 show that execution time is rapidly increase with increasing image size (total number of pixels). Data transfer time i.e., DRAM to GPU memory is considered for calculating the execution time. We can achieve average throughput of 5.67GB/s during memory transfer. The Execution Dependency stall reason occurs if an input dependency is not yet available due to bandwidth constraints. (Figure 5). The number of threads, grid size and block size used in the experiment are given in Table 1 and 2. We obtained approximately 6x speedup in this test and performance efficiency on GPU.

Table 1. Parallel execution MNDWI and SAVI

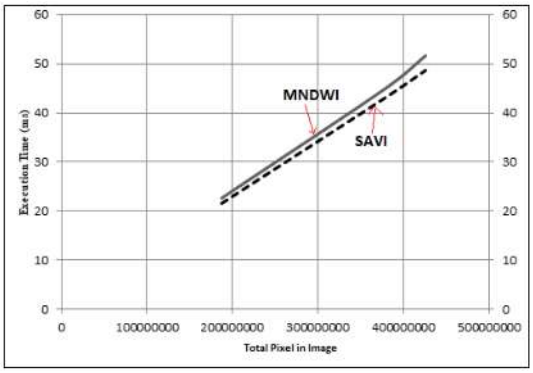
	Test Image 1	Test Image 2	Test Image 3
No of Pixels (Sample*Line)	14241 * 13191	20681*18271	14841*28641
Total Pixels	187853031	377862551	425061081
Execution Time (MNDWI) (ms)	23	45	52
Execution Time (SAVI) (ms)	21	43	49

Table 2. Serial execution MNDWI and SAVI

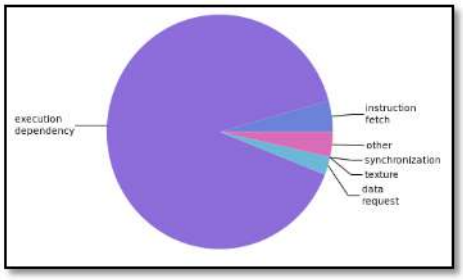
	Test Image 1	Test Image 2	Test Image 3
No of Pixels (Sample*Line)	14241 * 13191	20681*18271	14841*28641
Total Pixels	187853031	377862551	425061081
Execution Time (MNDWI) (ms)	2253	4669	4912
Execution Time (SAVI) (ms)	1302	3221	5749



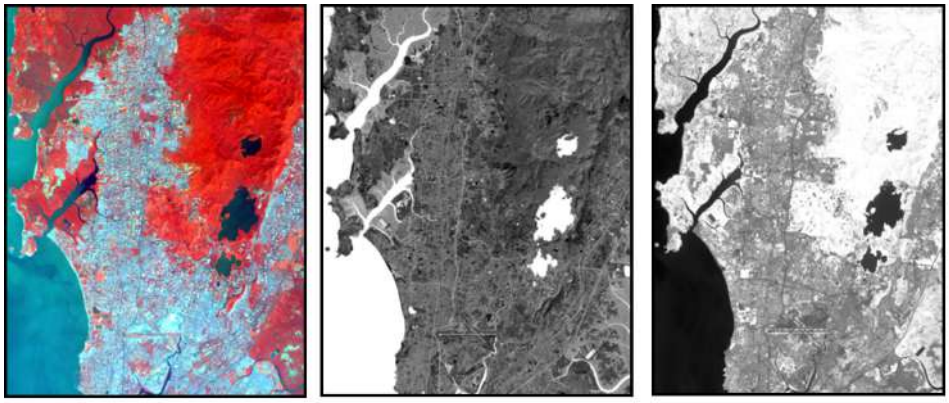
GPU parallel and serial computation performance of various test images



Comparison of execution time with number of pixels



Stall reasons pie chart show high execution dependency, it is because of bandwidth constraints. These long dependencies are typically caused by dependencies on global memory. Pie chart was derived using NVIDIA Visual Profiler



Sample input and output image of test area. Left image - FCC (Band: 5, 3, 1) of input Landsat- 8 OLI image; middle image - MNDWI output image, brighter pixels show water features (indices values range 0.17 to 0.325); right image - SAVI output image, brighter pixels show vegetation features (indices values range 0.46 to 0.81)

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work : Publication: Sivakumar V., Ankit. G., Biju C., (2021), Geospatial Information Extraction from Big Satellite Data using CUDA-enabled GPU Parallel Computing Technique, Journal of Geomatics, 15 (2), 152-159.

Journal of Geomatics Vol. 15, No. 2, October 2021

Geospatial Information Extraction from Big Satellite Data using CUDA-enabled GPU Parallel Computing Technique

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Abstract: Earth observational satellite images can provide massive quantities of data that in principle could be processed rapidly and provide valuable information to several domain specific applications. The Graphics Processing Unit (GPU) based parallel computation approach plays an important role in processing and analysing a large volume of satellite imageries and speed-up the computations. In the present paper, we implemented the indices computation algorithms i.e., Modified Normalized Difference Water Index (MNDWI) and Soil-Adjusted Vegetation Index (SAVI) for extracting useful information from satellite imagery using NVIDIA CUDA-enabled GPU's. We performed both parallel and serial approaches and compared the execution time and performances. Water and vegetation features were successfully delineated from multispectral LANDSAT – 8 satellite images. Performance result was compared with the conventional and GPU parallel computing approaches and achieved a speed up to ~6X on NVIDIA M2090 GPU. This experimental result shows that outputs can be achieved at high speed with the best utilization of GPU resources and an efficient parallelization approach. Result highlights that big data (larger area, resolution, size, etc) can be handled much easily with GPU parallel computing approach. This technique would be useful for the applications like natural resource monitoring, urban development, disaster management and agriculture.

Keywords: Geospatial, indices computation, parallel computing, NVIDIA-CUDA, GPU, MNDWI, SAVI

Title of the work carried out: Conformational Dynamics of Intrinsically Disordered and Ordered Protein

Name & Designation of the Chief Investigator: Dr. Sunita Patel (DST Women Scientist)

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Institution Name:UM-DAE Centre for Excellence in Basic Sciences, Mumbai

Application Domain: Chemical Scicences

Research Challenge/s: The main research challenges we faced are in scaling the replica exchange molecular dynamic simulation. The computational power are still not sufficient to achieve convergence.

Work carried, Milestone, Achievements & Graphs, Plots:

Uncloaking Self-association Sites in M-Crystallin Caused by Mutations Provide Insights of Cataract

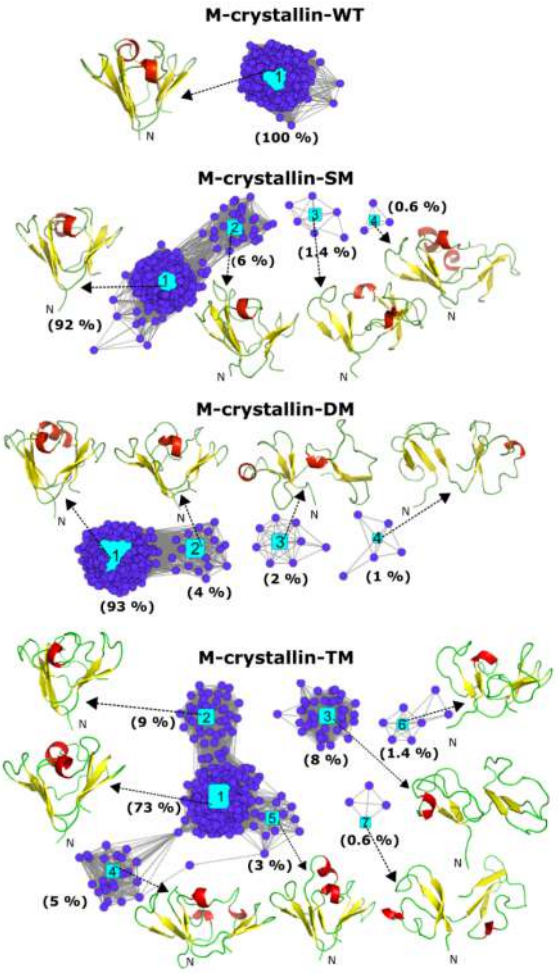
Cataract affects millions of people worldwide and is the leading cause of blindness in many developing counties. It happens by opacity in eye lens due to mutation in the crystallins leading to congenital cataract or due to post-translational modifcation, oxidative stress, exposure to UV radiation, heat, etc. causing age related cataract. WHO reported 2.2 billion people around the world to have vision impairment as of 2019. Of which 1 billion of cases could have been prevented by medical intervention1–3. Crystallins in the eye len constitute 90% of the total soluble proteins3 . A high concentration of soluble crystallins provide transparency and a high refractive index to the eye-lens4,5. Cataract is caused due to aggregation of eye lens crystallins which prevent light from reaching the retina5–7 . So far the molecular insights of the cause of cataract is not well understood.

In this study, we performed mutations at specifc sites of M-crystallin, a close homologue of eye lens crystallin and studied by using replica exchange molecular dynamics simulation. Mutations were made on the Ca2+ binding residues (K34D and S77D) and in the hydrophobic core (W45R) which is known to cause congenital cataract in homologous γD-crystallin. We generated single mutant of M-crystallin by mutating W45 to R45 and is abbreviated as M-crystallin-SM. Double mutant of M-crystallin was made by mutating K34D and S77D in the Ca2+ binding canonical motifs of M-crystallin and is referred as M-crystallin-DM. Similar way, triple mutant of M-crystallin was made by mutating K34D, W45R and S77D and is abbreviated as M-crystallin-TM using PyMOL software.

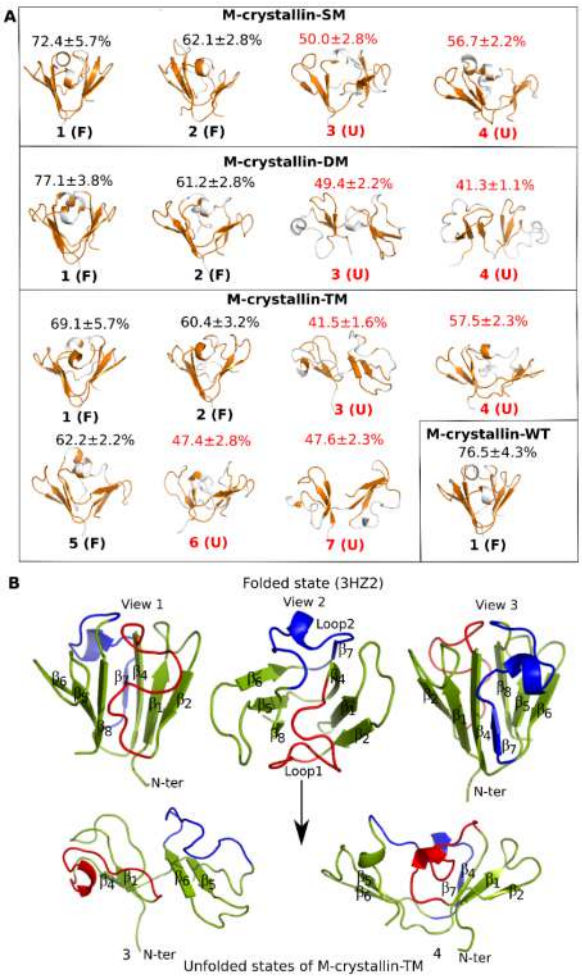
Conformational clusters observed in M-crystallin and its mutants

In the network analysis performed on REMD simulations showed a single cluster accounting 100% in M-crystallin-WT. The structures of the cluster are similar to the X-ray structure of M-crystallin suggesting retaintion of βγ-crystallin fold (Figure 1). In M-crystallin-SM where W45 residue is mutated to R45, 4 clusters were observed as shown in Figure 1. Cluster 1 has βγ-crystallin-like fold whereas cluster 2 has deformed loops but has -crystallin-like topology. The two minor clusters sample partially unfolded conformations where the central compact core is lost. In M-crystallin-DM, the network layout also shows four conformational clusters.. Cluster 1 and 2 have

βγ-crystallin-like fold while cluster 3 and 4 showed partially unfolded conformations. M-crystallin-TM shows seven conformational clusters. These clusters retain βγ-crystallin-like topology while cluster 3, 4, 6 and 7 are mostly in partially unfolded states (Figure 1). Some of the conformational clusters such as cluster 3 and 4 of M-crystallin-SM look similar to cluster 4 of M-crystallin-TM while cluster 3 and 4 of M-crystallin-DM are similar to cluster 3 and 7 of M-crystallin-TM. Overall, we observed βγ-crystallin-like ensemble for M-crystallin-WT while mixture of folded and partially unfolded conformational states for mutants.



Network cluster layouts of M-crystallin wild type and its mutants. An identical pairwise C□ RMSD cut-off of 3.5 Å was used for constructing these network layouts. Five hundred frames were taken at a regular interval from the equilibrated region (70-200 ns) of each simulations for this analysis. A centroid structure corresponding to each cluster is pointed by an arrow. Cytoscape version 3.5.1 (https://cytoscape.org/) is used to build network layout

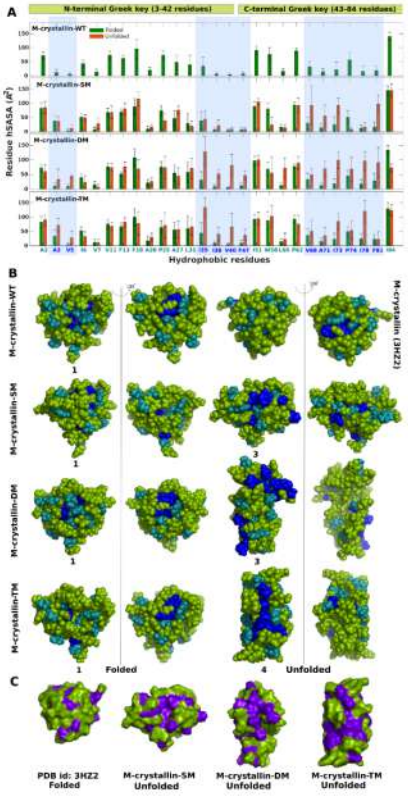


Native contact analysis was performed on the conformational clusters obtained from network cluster analysis. The average percentage of native contacts of a given cluster is indicated above the centroid structure (A). Clusters having 60% or greater native contacts are denoted as folded, F while the rest are designed as unfolded, U. In the centroid structures, the residues having native contacts are mapped in orange while rest of the residues are shown in white. (B) Three distinct views (one side view, top view, and opposite side view) of M-crystallin in X-ray structure are shown in top panel while unfolded representative states of M-crystallin-TM are shown in bottom panel. PyMol version 2.0.2 (https://pymol.org/2/) is used.

Segregation of conformational clusters into folded and unfolded states by native contact analysis

Native contact percentage is determined to segregate folded and unfolded conformation. If the percentage of native contact of a given cluster is more than 60%, it is considered as folded or else it is unfolded and are labelled as F and U respectively as shown Figure 2A. The single cluster of M-crystallin-WT possesses 76.5±4.3% of native contacts suggesting all the conformations are well folded and have βγcrystallin-like fold (Figure 2A). In M-crystallin-SM, out of four clusters, cluster 1 and 2 have 72.4±5.7 and 62.1±2.8% of native contacts and therefore are considered as folded while cluster 3 and 4 have 49.4±2.2 and 41.3±2.1% of native contacts thus are considered as unfolded (Figure 32). Similarly, in M-crystallin-DM out of four clusters cluster 1 and 2 are folded having 77.1±3.8 and 61.2±2.8% of native contacts while cluster 3 and 4 are unfolded hav-

ing 49.4±2.2 and 41.3±1.1% of native contacts. In M-crystallin-TM, cluster 1, 2 and 5 possess 69.1±5.7, 60.4±3.2 and 62.2±2.2% of native contacts respectively and therefore are folded while clusters 3, 4, 6 and 7 are having 41.5±1.6, 57.5±2.3, 47.4±2.8 and 47.6±2.3% of native contacts respectively and therefore are unfolded clusters (Figure 2A). Native contact analysis reveals that the observed unfolded states possess 40-50% of native contacts and thus are not completely unfolded like random coil but are partially unfolded states.



The average hydrophobic solvent accessible surface area per residue is determined for the folded or unfolded states in all simulations. For this calculation all the folded and unfolded clusters are combined and made into two separate groups. rhSASA of folded and unfolded groups are determined and are shown in bar plots (A). The light blue shaded boxes indicate the residues with higher hydrophobic exposure in unfolded states. These residues are mapped on the centroid structure (cluster number indicated below the centroid structure) in blue van der Waals spheres, the rest hydrophobic residues in cyan and residues other than the hydrophobic residues are in green color (B). Two color codes are used to indicate hydrophobes (purple) and nonhydrophobes (green) to indicate the hydrophobic patches (C). MATLAB R2017b (https://in.mathworks.com/) is used for the hSASA plots. PyMol version 2.0.2 (https://pymol.org/2/) is used to show hydrophobic surface area.

Large hydrophobic solvent accessible surface area displayed by unfolded states:

The residue specific solvent accessible surface area (rhSASA) is estimated for folded (F) and unfolded (U) conformational states of a given simulation which are grouped based on their native contact percentage (Figure 2A). In M-crystallin-SM, the rhSASA of the residues V68, A71, I73 and F81 are relatively more exposed in unfolded state compared to its folded counterpart (Figure 3A). These residues are located in the loop2 region of C-terminal Greek key. Similarly, in M-crystallin-DM hydrophobic exposure is observed in the similar region corresponding to the residues L60, V68, A71, I73, I78 and F81. In addition, there are two more regions corresponding to the residues I35, I38, V40 and F47 located at the junction of N- and C-terminal Greek keys and residues A3 and V5 of N-terminal Greek key are showing higher values of rhSASA in the partially unfolded states compared to that of folded state. Similarly, in M-crystallin-TM similar regions as observed in M-crystallin-DM are exposed (Figure 3). These residues showing higher values of rhSASA in the unfolded state are mapped onto the centroid structure of folded and unfolded clusters as shown in Figure 3B. There is a remarkable difference in the hydrophobic surface exposure of a folded and unfolded conformations. The folded conformations from wild type, mutants and X-ray structure show, a significant burial of hydrophobic residues while on the partially unfolded states there is conspicuous exposure of hydrophobic residues which form continuous hydrophobic patches of the size 500 to 700 Å2 (Figure 3C). These sites can act as attachment sites for self-aggregation into higher molecular weight aggregates and thus can lead to cataract in homologous eye-lens crystallins.

In our REMD simulations M-crystallin-WT does not show any dramatic conformational change because of optimal packing of hydrophobic residues in the core, and presence of several interlocking Greek key interactions. On the other hand in all mutants of M-crystallin, formation of heterogeneous mixture of folded and partially unfolded states are observed. The partially unfolded states are mainly of two types. In one type, the two Greek key motifs are apart without any significant interactions between the two Greek keys while in second type, the central hydrophobic core is largely perturbed and the compact core is lost but still held by several interactions from both the Greek keys. In either types of unfolded states, the buried hydrophobic residues are exposed giving rise to large hydrophobic patches. These hydrophobic patches are mainly contributed by the hydrophobic residues located at the junction of both Greek keys and at the C-terminal Greek key motif. These hydrophobic patches can provide attachment sites for association into higher order molecular aggregates. Thus, hydrophobic patches on the partially unfolded crystallin are the main determinant of βγ-crystallin aggregation. Interactions restricting the loop dynamics and promoting the strength of hydrophobic core can reduce the hydrophobic exposure and thus can prevent the aggregation of crystallin which is the main cause of cataract.

References:

1. Organization, W. H. World report on vision. https://www.who.int/publications-detail/world-report-on-vision (2019).

2. Resnikof, S. et al. Global data on visual impairment in the year 2002. Bull. World Health Organ. 82, 844–851 (2004).

3. Pescosolido, N., Barbato, A., Giannotti, R., Komaiha, C. & Lenarduzzi, F. Age-related changes in the kinetics of human lenses: Prevention of the cataract. Int. J. Ophthalmol. Clin. Res. 9, 1506–1517 (2016).

4. Zhao, H., Magone, M. T. & Schuck, P. Te role of macromolecular crowding in the evolution of lens crystallins with high molecular refractive index. Phys. Biol. 8, 046004 (2011).

5. Roskamp, K. W., Paulson, C. N., Brubaker, W. D. & Martin, R. W. Function and aggregation in structural eye lens crystallins. Acc. Chem. Res. 53, 863–874 (2020).

6. Mahler, B. et al. Characterization of a transient unfolding intermediate in a core mutant of γs-crystallin. J. Mol. Biol. 405, 840–850 (2011).

7. Serebryany, E. & King, J. A. Te βγ-crystallins: Native state stability and pathways to aggregation. Prog. Biophys. Mol. Biol. 115, 32–41 (2014).

Benefits & experience of using NPSF:

We performed molecular dynamics simulation using NPSF PARAM Yuva-II system. Although, it was slow however we could achieve the required simulation length by using it for longer time.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work:

1. **More number of cores with good computing power should be offered.**
2. **Wall time should be more for users.**

Work Report 5 Summary

Title of the work carried out: Different kinds of energy conversion in 2D materials via first principles-based approach.

Name & Designation of the Chief Investigator: Prof. Dr. Abir De Sarkar, Scientist-F/Professor and Dean (Academics)

E-mail Id:abir@inst.ac.in, abirdesarkar@gmail.com

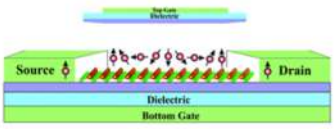
Institution Name: Institute of Nano Science and Technology (Autonomous Institute supported by the Department of Science and Technology, Government of India), Sector-81, Knowledge City, Manauli, SAS Nagar, Mohali, Punjab - 140306

Application Domain: Computational Nanoscience: Physics & Material Sciences

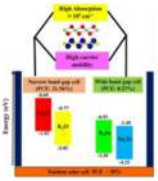
Research Challenge/s: Studying systems having a large number of atoms, which can be highly computationally intensive and demanding & also running some calculations, such as, molecular dynamics simulations, for a long duration of time (say, more than 80 hrs) .

Work carried, Milestone, Achievements & Graphs, Plots:

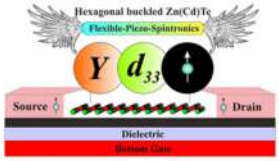
Conflux of tunable Rashba effect and piezoelectricity in flexible magnesium monochalogenide monolayers for next-generation spintronic devices
Nanoscale, 2021, 13, 8210-8223



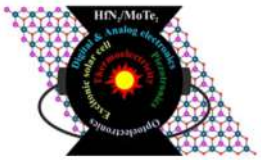
Interfacing 2D M2X (M = Na, K, Cs; X= O, S, Se, Te) monolayers for 2D excitonic and tandem solar cells
Applied Surface Science, 2021, 563, 150304



Spin-current modulation in hexagonal buckled ZnTe and CdTe monolayers for self-powered flexible-piezo-spintronic devices
ACS Appl. Mater. Interfaces, 2021, 13, 34, 40872-40879



Atomistic manipulation of interfacial properties in HfN2/MoTe2 van der Waals heterostructure via strain and electric field for next generation multifunctional nanodevice and energy conversion
Applied Surface Science 2021, 568, 150928



Chem Soc Rev

REVIEW ARTICLE

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A bright future for engineering piezoelectric 2D crystals

Peter C. Sherrell, Marco Fronzi, Nick A. Shepelin, Alexander Corletto, David A. Winkler, Mike Ford, Joseph G. Shapter and Amanda V. Ellis

ROYAL SOCIETY OF CHEMISTRY

Piezoelectricity in heterostructures from dissimilar 2D crystals was first predicted by Mohanta *et al.* for GaN/boron monophosphide crystals.[83] These heterostructures were predicted to have a d_{33} of up to 40 pm V^{-1}. Subsequent predictions have shown that 2D crystal heterostructures with large out-of-plane piezoelectricity can be produced using constituent 2D crystals that only possess in-plane piezoelectricity.[84,85]

Recent works using computational approaches, led by Abir De Sarkar, have reported that applied strains may induce ultra-high, colossal, or gigantic out-of-plane piezoelectricity to Janus 2D crystals.[107,110,111] These results, obtained using DFT,

Publications:

1. Manish Kumar Mohanta, Anu Arora, Abir De Sarkar* (2021). "Conflux of tunable Rashba effect and piezoelectricity in flexible magnesium monochalogenide monolayers for next-generation spintronic devices". Nanoscale, 2021, 13, 8210-8223 (Impact factor: 7.790)

2. Ashima Rawat, Anu Arora, Abir De Sarkar* (2021). "Interfacing 2D M2X (M = Na, K, Cs; X= O, S, Se, Te) monolayers for 2D excitonic and tandem solar cells". Applied Surface Science 563, (2021) 150304 (Impact factor: 6.707)

3. Ashima Rawat, Dimple, Raihan Ahammed, Abir De Sarkar* (2021). "Concurrence of negative in-plane piezoelectricity and photocatalytic properties in 2D ScAgP2S6 monolayers". J. Phys.: Condens. Matter 33 (2021) 375301 (Impact factor: 2.333)

4. Manish Kumar Mohanta, Ashima Rawat, Abir De Sarkar* (2021). "Atomistic manipulation of interfacial properties in HfN2/MoTe2 van der Waals heterostructure via strain and electric field for next generation multifunctional nanodevice and energy conversion". Applied Surface Science 2021, 568, 150928 (Impact factor: 6.707)

5. Manish Kumar Mohanta, Fathima IS, Amal Kishore, Abir De Sarkar* (2021). "Spin-current modulation in hexagonal buckled ZnTe and CdTe monolayers for self-powered flexible-piezo-spintronic devices". ACS Appl. Mater. Interfaces 2021, 13, 34, 40872–40879 (Impact factor: 9.229)

6. Manish Kumar Mohanta, Anu Arora, Abir De Sarkar* (2021). "Effective modulation of ohmic contact and carrier concentration in a graphene-MgX (X = S, Se) van der Waals heterojunction with tunable band-gap opening via strain and electric field". Phys. Rev. B 104, 165421 (Impact factor: 4.036)

7. Group-IV(A) Janus dichalcogenide monolayers and their interfaces straddle gigantic shear and in-plane piezoelectricity" Pradip Nandi, Ashima Rawat, Raihan Ahammed, Nityasagar Jena, Abir De Sarkar*, Nanoscale, 2021,13, 5460-5478(Impact factor: 7.790)

8. Manish Kumar Mohanta, Harshita Seksaria, Abir De Sarkar* (2022). "Insights into CrS2 monolayer and n-CrS2/p-HfN2 interface for low-power digital and analog nanoelectronics". Applied Surface Science, 579, 30 March 2022, 152211 (Impact factor: 6.707)

9. Raihan Ahammed and Abir De Sarkar* (2022). "Valley spin polarization in two-dimensional h-MN (M= Nb, Ta) monolayers: Merger of valleytronics with spintronics". Phys. Rev. B 105 (2022) 045426 (Impact factor: 4.036)

Recognition:

Pioneering findings of our group have been duly recognized and cited in the RSC journal Chem. Soc. Rev. 2022, 51, 650-671 (Impact factor 54.56) and featured as Editor's choice in Nanoscale

Chem Soc Rev

REVIEW ARTICLE

View Article Online

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A bright future for engineering piezoelectric 2D crystals

Peter C. Sherrell, Marco Fronzi, Nick A. Shepelin, Alexander Corletto, David A. Winkler, Mike Ford, Joseph G. Shapter and Amanda V. Ellis

ROYAL SOCIETY OF CHEMISTRY

Piezoelectricity in heterostructures from dissimilar 2D crystals was first predicted by Mohanta *et al.* for GaN/boron monophosphide crystals.[83] These heterostructures were predicted to have a d_{33} of up to 40 pm V^{-1}. Subsequent predictions have shown that 2D crystal heterostructures with large out-of-plane piezoelectricity can be produced using constituent 2D crystals that only possess in-plane piezoelectricity.[84,85]

Recent works using computational approaches, led by Abir De Sarkar, have reported that applied strains may induce ultra-high, colossal, or gigantic out-of-plane piezoelectricity to Janus 2D crystals.[107,110,111] These results, obtained using DFT,

Our article titled 'Superhigh out-of-plane piezoelectricity, low thermal conductivity and photocatalytic abilities in ultrathin 2D van der Waals heterostructures of boron monophosphide and gallium nitride' published in Nanoscale 11 (2019) 21880-21890 has been specially selected to feature in an Editor's Choice web collection focussing on computational nanomaterials research under the theme Computational studies of nanomaterials for energy, catalysis and electronics .

Benefits & experience of using NPSF:

PARAM Yuva II is immeasurably helping the Ph.D. students of my research group on a wide range of research problems. We are able to carry forward the computational research work with ease through these resources.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work :

PARAM Yuva-II is doing a magnificent job in providing computational resources to pursue scientific research. We wish for more access of resources for advancing the research for some long duration calculations like molecular dynamics simulations (requiring more than 80-90 hrs).

Title of the work carried out:

(a) Inhibitors of Plasmepsin X Plasmodium falciparum: Structure-based pharmacophore generation and molecular dynamics simulation

(b) Inhibitors of Heptosyltransferase I to prevent heptose transfer against antibiotic resistance of E. coli: Energetics and stability analysis by DFT and molecular dynamics

Name & Designation of the Chief Investigator: Malay Kumar Rana, Assistant Professor

E-mail Id:mrana@iiserbpr.ac.in

Institution Name: Indian Institute of Science Education and Research Berhampur (IISER Berhampur)

Application Domain: Bio Sciences, Bioinformatics, and Chemical Sciences

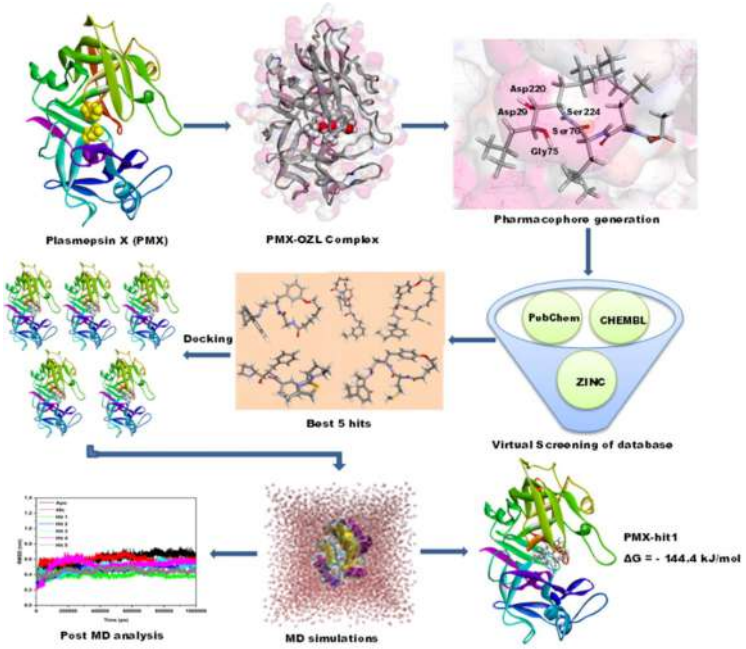
Research Challenge/s:

(a) Among Plasmodium parasites, Plasmodium falciparum is the most effective for malaria infection. Plasmepsin X (PMX), an aspartic protease, plays an important role in egress and invasion of the parasite in the intraerythrocytic stage. The lack of X-ray crystal structure of PMX prohibits the discovery of potential PMX inhibitors. With the homology modelling of PMX, we have identified potential inhibitors from various databases through docking, virtual screening and molecular dynamics in this study.
(b) Heptosyltransferase I (HEP I) helps in the synthesis of lipopolysaccharide (LPS) by adding heptose sugars to the inner core of Gram-negative bacteria, e.g., Escherichia coli. LPS biosynthesis causes bacterial infections and antibiotic resistance. Thus, the interruption LPS biosynthesis is inevitable to prevent bacterial infections caused by E. coli. In this context, we have searched for HEP I inhibitors by computational methods to stop bacterial infections.

Work carried, Milestone, Achievements & Graphs, Plots:

(a) Malaria is a life-threatening disease caused by Plasmodium parasites, which are transmitted to humans through infected female Anopheles mosquitoes. Over the past few decades, antimalarial resistance has posed one of the most important health challenges around the globe. To counteract the increased resistance to artemisinin combination therapy (ACT), the discovery of effective new antimalarial medicines is required at the moment. Plasmepsin X (PMX), an aspartic protease, is unravelled recently for playing an important role in egress and invasion of intraerythrocytic parasites by activating subtilisin-like protease 1. Therefore, the current study is centralized on PMX for in-silico identification of effective drugs. Structure based pharmacophore generation and virtual screening filtered out 47 candidates from almost 108 million entries catered in CHEMBL, PubChem, and ZINC databases. Five best hits were chosen based on docking scores. 1 µs molecular dynamics of homologue PMX and its complexes with the shortlisted five hit molecules and a known inhibitor 49c elucidated the stability of the complexes. Consistent with docking, the binding free energy estimated using MM-PBSA method recognized hits 1 (144.4 kJ/mol) and 2

(130.1 kJ/mol) the best inhibitors among all hits and the known inhibitor 49c (68.7 kJ/mol). The new inhibitors can be put forward for further in-vivo studies as an antimalarial drug based on the comprehensive analyses reported herein.

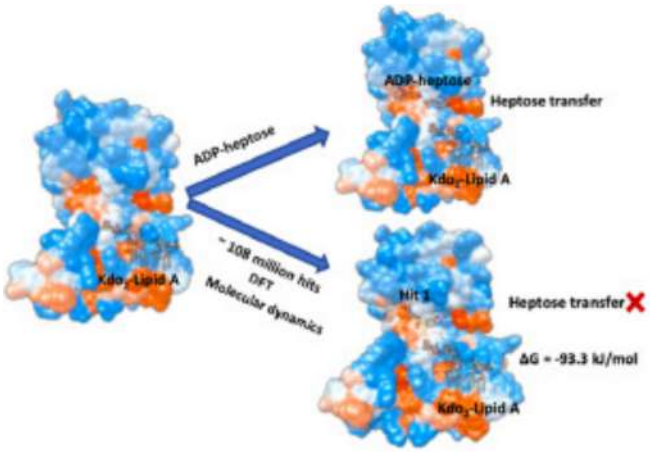


A scheme for screening potential PMX inhibitors.

(b) Heptosyltransferase I (HEP I) belongs to the broad family of glycosyltransferase-B (GT-B) enzymes, which transfers heptose sugar necessary for the lipopolysaccharide (LPS) synthesis. LPS is a significant component of the external cell membrane of Gram-negative bacteria, e.g., Escherichia coli. Interruption of heptose sugar addition during LPS biosynthesis greatly reduces bacterial infections and antibiotic resistance. Thus, inhibition of HEP I is indispensable to counteract this problem. Here, we have performed virtual screening employing structure-based pharmacophore, docking, pharmacokinetics, and electronic descriptors to identify four important hit molecules from a pool of

$\approx$

108 million bioactive molecules existing in ZINC, PubChem, and CHEMBL databases against HEP I. Pharmacokinetics and all electronic descriptors describing the bioavailability of the selected hits fall within the permissible limits. Further, molecular dynamics simulations of the shortlisted hits along with a reference molecule discern the conformational stability of the bound complexes, characterized by RMSD, RMSF, Rg, SASA, and PCA. The large negative MM-PBSA-based binding free energy validates the initial screening results and hence the inhibitory potential of the hits. The study suggests that the best three candidates, hit 1 (CHEMBL1438912), hit 3 (CHEMBL13895), and hit 4 (CHEMBL320880), can be very promising to retard the heptose sugar transfer and eradicate the antibiotic resistance of E. coli, providing molecular insights into the inhibition of HEP I. This may facilitate further in-vitro studies of the best hits and targeted antibacterial drug development.



Inhibition of HEP I.

Benefits & experience of using NPSF:

Param Yuva II has been very useful for the aforementioned research. Thanks to the staff who have been very helpful in resolving any technical issues whenever needed.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : The cluster seems to be a bit sluggish to run molecular dynamics for systems of large size, typically for large proteins. (Although this may depend on a variety of factors, we believe we can optimize further.)

Publication:

1. "Inhibitors of Plasmepsin X Plasmodium falciparum: Structure-based pharmacophore generation and molecular dynamics simulation", Panda, S. K., Saxena, S., Sen Gupta, P. S. & Rana, M. K., Journal of Molecular Liquids, 116851, 2021. Impact Factor: 6.165. (doi: 10.1016/j.molliq.2021.116851)

2. "Inhibitors of Heptosyltransferase I to prevent heptose transfer against antibiotic resistance of E. coli: Energetics and stability analysis by DFT and molecular dynamics", Bhattacharya, U., Panda, S. K., Sen Gupta, P. S. & Rana, M. K., Journal of Molecular Structure, 1253, 132258, 2022. Impact Factor: 3.196. (doi: 10.1016/j.molstruc.2021.132258)

Work Report 7 Summary

Title of the work carried out: Thermoelectric behavior of KCuS monolayer.

Name & Designation of the Chief Investigator: Subhasmita Kar, PhD Scholar at IIT Patna

E-mail Id:subhasmita_1921ph02@iitp.ac.in

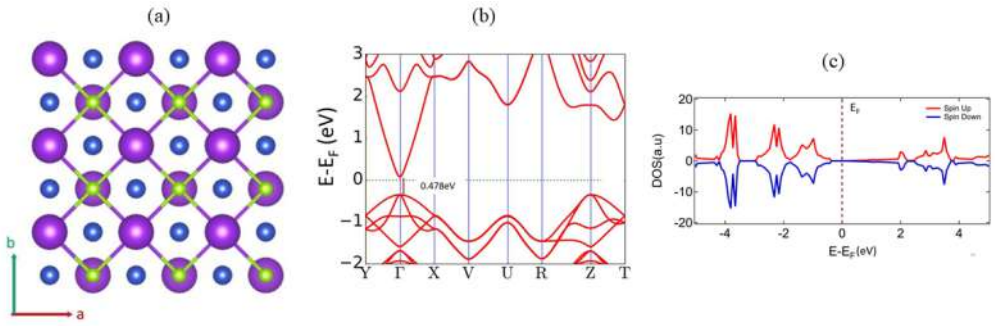
Institution Name: Indian Institute of Technology Patna

Application Domain: Computational Physics

Research Challenge/s: My project is based on Density Functional Theory (DFT) calculations. And some DFT calculations are highly computational expensive and time consuming . So the challenge is to solve large systems in order to understand the behavior of materials.

Work carried, Milestone, Achievements & Graphs, Plots:

We have performed Density Functional Theory (DFT) based calculations to explore the electronic and thermoeletric properties of KCuS monolayer. The 2D KCuS is a direct bandgap semiconductor with a value of 0.47 eV.



(a) The top view (Purple: K, Blue: Cu, Yellow: S), (b) spin polarized band structure and (c) density of states (DOS) of KCuS monolayer.

Benefits & experience of using NPSF:

I can able to run my expensive calculations by using NPSF PARAM Yuva-II

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : It would be more beneficial for me If I can get more time to run my calculations.

Work Report 8 Summary

Title of the work carried out: Quantum_Hall-PR

Name & Designation of the Chief Investigator: Sreejith GJ , Associate Professor

E-mail Id:anand.abhishek@students.iiserpune.ac.in

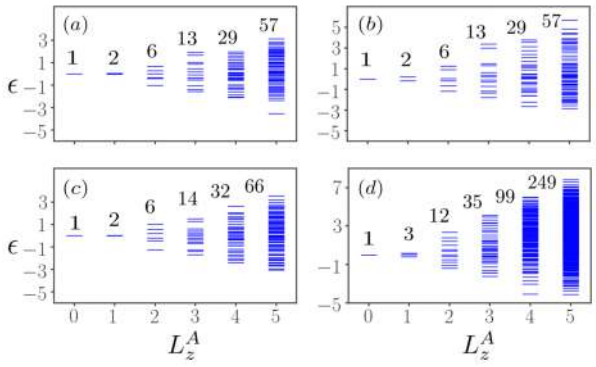
Institution Name: Department of Physics, IISER Pune

Application Domain: Computational Condensed matter physics

Research Challenge/s: Apart from the long queue wait, there was no other challenge.

Work carried, Milestone, Achievements & Graphs, Plots:

A part of overlap calculations in the project were done on Yuva. These spectra of the overlap tell topological features of the Hall wavefunctions.



Benefits & experience of using NPSF:

During the early period of my research, when IISER was lacking HPC systems, Yuva provided the means to do parallel calculations, helping finish the projects on time. I thank CDAC for waiving the fee and providing the timely resource.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work :

None.

Title of the work carried out: Numerical simulations of hydromagnetic turbulence from galaxies to the Sun

Name & Designation of the Chief Investigator: Dr. Sharanya Sur, Associate professor

E-mail Id:piyali.chatterjee@iiap.res.in

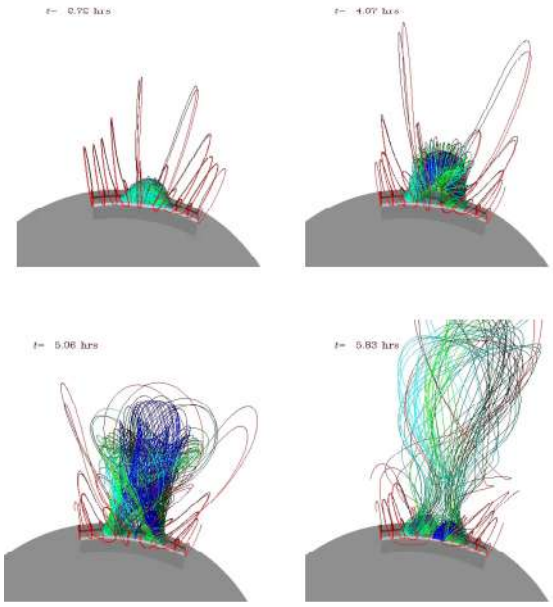
Institution Name: Indian Institute of Astrophysics

Application Domain: Astronomy & Astrophysics

Research Challenge/s: Queue waiting time ¿ 2 days for 256-512 processors even for 2 hour testq. This makes testing very challenging.

Work carried, Milestone, Achievements & Graphs, Plots:

Work in progress on solar Coronal Mass Ejection initiation: Our fully compressible MHD set-up in spherical geometry studies the evolution of the magnetic field in the corona with a grid size of 512X160X288 in r, theta and phi directions as a result of quasi-statically emerging a part of a highly twisted torus through the lower boundary into a pre existing coronal potential field. We allow this system to evolve following the set of magneto-hydrodynamic equations comprising of mass conservation, Navier-Stokes, Faraday's induction equation and the energy equation. We have now ported the set-up to the open source MPI parallel Pencil Code (http://pencil-code.nordita.org) which is a multi-user, cache efficient higher-order finite difference code. Additionally, we have now incorporated (and tested) new physics like the semi relativistic Boris correction, anisotropic heat transport along field lines (Spitzer conductivity), and optically thin radiative cooling into our set-up. In the adjoining figure, we show some initial results from the set-up where we see a flux rope eruption in form of a CME due to torus+kink instability.



Different stages of magnetic flux rope erupting in the solar corona due to ideal MHD instabilities. The times since the start of simulation are indicated in the panels. The red field lines denote the pre existing coronal field. The green/cyan/blue lines indicate the field lines from outer to inner part of the emerging flux rope.

With the Aditya-L1 mission launching hopefully in 2023, such theoretical studies done indigenously in India would be important in understanding the dynamics of the corona along with the observations made by the VELC and SUIT instruments on board Aditya-L1.

Benefits & experience of using NPSF:

Presently, I am combining computing time available on Param Yuva II with local HPC to carry out code testing. It is very helpful since I can test more cores (¿ 512) on Param Yuva which I cannot do on my Institute's local HPC.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : very slow on the existing sandy bridge processors. Even though it runs reasonably fast (10X) on broadwell and above processors. I do not know if it is the specific communication fabric or processor.

Title of the work carried out:

1. Dissolution of Caffeine Crystal in Supercritical CO2 Ethanol Solution

2. CelS-catalyzed Processive Cellulose Degradation and Cellobiose Extraction for Production of Bioethanol

Name & Designation of the Chief Investigator: Dr. Moumita Saharay, Assistant Professor

E-mail Id:moumitasaharay@uohyd.ac.in

Institution Name: Department of Systems and Computational Biology, School of Life Sciences, University of Hyderabad, Gachibowli, Hyderabad

Application Domain: Atomic and molecular Sciences, Computational Physics

Research Challenge/s: Waiting time in the job queue is too long.

Work carried, Milestone, Achievements & Graphs, Plots:

Two manuscripts have been submitted to peer review journals.

Benefits & experience of using NPSF:

I could use multiple processors to speed up my jobs. Thanks to NPSF PARAM Yuva-II. But, sometimes the waiting time in the job queue is too long.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work : None

Title of the work carried out: Optoelectronic and Photocatalytic Properties of Stable Pentagonal B2S and B2Se Monolayers

Name & Designation of the Chief Investigator: Dr. Jagdish Kumar, Assistant Professor in Department of Physics and Astronomical Science, Central University of Himachal Pradesh, Dharamshala

E-mail Id:jagdish@cuhimachal.ac.in , nehakatoch2@gmail.com

Institution Name: Central University of Himachal Pradesh, Dharamshala.

Application Domain: Condensed Matter Physics: Materials Modeling using DFT

Research Challenge/s: Novel Two-Dimensional Structures beyond Graphene: A First Principle Study

Work carried, Milestone, Achievements & Graphs, Plots:

We have carried out DFT based study of optoelectronic and photocatalytic properties of stable Pentagonal B2S and B2Se monolaters. Stabilities of these monolayers have been checked. Results reveal that these monolayers possess a moderate bandgap, high hole mobility, strong optical absorption in the visible region and strain-induce indirect-to-direct bandgap transition. Furthermore, these monolayers can be useful for photocatalytic water splitting under suitable strain and solution conditions. Our predicted results make these monolayers to be candidate materials for optoelectronic and photocatalytic applications.

Benefits & experience of using NPSF:

It's a nice experience of using NPSF and quick response of querries. During pandemic NPSF was a major support.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : No

Title of the work carried out: Role of functionalised g-ZnO and g-GaN nanosheets in Optoelectronic devices : A Firstprinciples study.

Name & Designation of the Chief Investigator: Dr. Jagdish Kumar, Assistant Professor in Department of Physics and Astronomical Science, Central University of Himachal Pradesh, Dharamshala

E-mail Id:sandhya.wakhare@yahoo.co.in

Institution Name:HPT Arts and RYK Science college, Nashik, Maharashtra, India.

Application Domain: Computational Physics

Research Challenge/s: It is challenging to run the large electron system with high k-points with optimal speed and time.

Work carried, Milestone, Achievements & Graphs, Plots:

"The structural, electronic and optical properties of in-doped ZnO monolayer: A first principles study", AIP Conference Proceedings 2335, 080013 (2021); https://doi.org/10.1063/5.0046130.

Benefits & experience of using NPSF:

High supercomputing facility improved the work efficiency and speed of execution of programs.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : PARAM Yuva-II provides an excellent facility to researchers.

Title of the work carried out: Optimizing the morphological, electric and electrochemical properties of TiO_2 , Polythiophene and PEDOT: PSS films and the junctions between them for use in Supercapacitors

Name & Designation of the Chief Investigator: Prof. Ashish B. Chourasia

E-mail Id:vishallonikar@gmail.com (User-Other than CI)

Institution Name:HPT Arts and RYK Science college, Nashik, Maharashtra, India.

Application Domain: Material Sciences

Research Challenge/s: NA

Work carried, Milestone, Achievements & Graphs, Plots:

NA

Benefits & experience of using NPSF:

NA

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : NA

Title of the work carried out: Study of evolution of magnetism in the defected graphene

Name & Designation of the Chief Investigator: Prof. Anindya Datta (Professor)

E-mail Id:anindya.datta@ipu.ac.in

Institution Name: Guru Gobind Singh Indraprastha University, Dwarka Sector 16 C, New Delhi 110078

Application Domain: Computational Physics/ Material Sciences

Research Challenge/s: The challenge we are facing is to have difference in results obtained earlier using the facilities of IUAC. We are working on to resolve the difference through changing the approximation/potential.

Work carried, Milestone, Achievements & Graphs, Plots:

The major objective of the proposed work is to study the graphene and other 2D materials in presence of the defects using Density Functional Theory (DFT). Defects can introduce various functionalities in the systems but upto a certain limit after that the structure may transform to some other structures and properties may be lost.
We have studied the monolayer of zigzag graphene (with 54 atoms) with one and two defects using VASP code. It was found that onset of ferromagnetism takes place on introducing a few defect(s) and on further increasing the defects, the magnetism gets diminished and structure of graphene gets amorphous. As an extension of the work, we are planning to increase the number and size of graphene sheet to get more insight to justify the results and to examine the limit of amorphosization.

Benefits & experience of using NPSF:

For the simulation, we have run the code with 128 cpus and job was converged well in time. The same was taken comparatively long time other servers. In this way, it is really appreciable to have such a National facility to continue the research work. Earlier we have been using the facilities from IUAC, New Delhi. We don't have comparative data at the moment but certainly the NPSF facilities are much supirier and support system is very good.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : We found that working with the NPSF team is very appreciable. We have started last year but due to Covid, the student involvement was low. However, if solved, this problem will throw new light about magnetism in Graphene, which is directly dependent on this facility and its efficiency.

Title of the work carried out:RNA-Duplex , Ecoli_Structure

Name & Designation of the Chief Investigator: Thenmalarchelvi Rathinavelan, Asscoiate Professor

E-mail Id:tr@iith.ac.in

Institution Name: Indian Institute of Technology Hyderabad

Application Domain: Bio Sciences/ Bioinformatics

Research Challenge/s: NIL.

Work carried, Milestone, Achievements & Graphs, Plots:

1. P. P. Uttamrao, C. Sathyaseelan*, L. P. P. Patro*, T. Rathinavelan, "Revelation of potent epitopes present in unannotated ORF antigens of SARS-CoV-2 using immunoinformatics approach for the polyvalent epitope vaccine design". Frontiers in Immunology, doi.org/10.3389/fimmu.2021.692937

2. Patro, L.P.P.*, Sathyaseelan, C.*, Uttamrao, P.P.* and Rathinavelan, T. (2021), "Global variation in SARS-CoV-2 proteome and its implication in pre-lockdown emergence and dissemination of 5 dominant SARS-CoV-2 clades" . Infection, Genetics and Evolution., doi.org/10.1016/j.meegid.2021.104973.

3. Patro, L.P.P.*, Sathyaseelan, C.*, Uttamrao, P.P.* and Rathinavelan, T. (2021), "The evolving proteome of SARS-CoV-2 predominantly uses mutation combination strategy for survival" . Comput Struct Biotechnol J., doi: 10.1016/j.csbj.2021.05.054.

4. Sathyaseelan, C.*, Vijayakumar, V.* and Rathinavelan, T. (2021), "CD-NuSS: A Web Server for the Automated Secondary Structural Characterization of the Nucleic Acids from Circular Dichroism Spectra Using Extreme Gradient Boosting Decision-Tree, Neural Network and Kohonen Algorithms" . J Mol Biol., 433(11):166629. doi.org/10.1016/j.jmb.2020.08.014

5. Ajjugal, Y.*, Kolimi, N.* and Rathinavelan, T. (2021), "Secondary structural choice of DNA and RNA associated with CGG/CCG trinucleotide repeat expansion rationalizes the RNA misprocessing in FXTAS" . Sci Rep., 11(1):8163. doi.org/10.1038/s41598-021-87097-y

6. Ajjugal, Y.*, and Rathinavelan, T. (2021), "Sequence dependent influence of an A... A mismatch in a DNA duplex: An insight into the recognition by hZαADAR1 protein" . J Struct Biol., 213(1):107678. doi.org/10.1016/j.jsb.2020.107678

7. Ajjugal, Y.*, Tomar, K.* Rao, D.K., and Rathinavelan, T. (2021), "Spontaneous and frequent conformational dynamics induced by A... A mismatch in d (CAA)· d (TAG) duplex" . Sci Rep., 11(1):3689. doi.org/10.1038/s41598-021-82669-4

8. Ajjugal, Y.*, and Rathinavelan, T. (2021), "Conformational distortions induced by periodically recurring A... A in d (CAG). d (CAG) provide stereochemical rationale for the trapping of MSH2. MSH3 in polyQ disorders"Computational and structural biotechnology journal 19, 4447-4455

Benefits & experience of using NPSF:

By providing the computational resources

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : N/A

Title of the work carried out: First-Principle Study of the Electronic Structures of Heterostructure Devices and Their Related Applications.

Name & Designation of the Chief Investigator: Dr. Anver Aziz (Associatet Professor)

E-mail Id:mohammad159027@st.jmi.ac.in

Institution Name: Jamia Millia Islamia, New Delhi

Application Domain: Computational Physics, Material Sciences and Li-ion batteries

Research Challenge/s: Wall time is too short for large Phonon calculations .

Work carried, Milestone, Achievements & Graphs, Plots:

We have published two papers in peer-reviewed journals. List of publications during this period is given below:

1. Mohammad Ubaid, A Aziz, BS Pujari, "Two-dimensional C3N/blue phosphorene vdW heterostructure for Li, Na and K-ion batteries", New J. Chem., (45) 2021 12647–12654.
2. S Imam, KS Bayikadi, Mohammad Ubaid et al., "Achieving synergistic performance through highly compacted microcrystalline rods induced in Mo doped GeTe based compounds", Materials Today Physics, (2) 2022, 100571.

Benefits & experience of using NPSF:

Our experience of using NPSF is great. Due to NPSF, we are able to do expensive calculations in a very short time. We wish to thank National NPSF for providing the computation facility by PARAM Yuva II cluster.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : We appreciate your comments/feedback/suggestions to improve our system.

Title of the work carried out: Computational studies on Surface enhanced Raman spectra of biomolecules adsorbed on gold and silver nanoclusters for exploration of biosensing applications

Name & Designation of the Chief Investigator: Dr. N. V. Suresh Kumar, Assistant Professor of Physics

E-mail Id:surshkumar_nv@vnrvjiet.in

Institution Name:VNR Vignana Jyothi Institute of Engineering and Technology – Hyderabad

Application Domain: Atomic and Molecular Sciences and Computational Chemistry

Research Challenge/s: The computational facilites of NPSF PARAM Yuva-II are easy to access and run the simulations. If any problem comes, the help team responds to the mail/phone contact, and solves the problem.

Work carried, Milestone, Achievements & Graphs, Plots:

My project got approved in December 2021. The work is in progess.

Benefits & experience of using NPSF:

I could able to run electronic structure theory calcualtions using GAMESS and Qauntume-spresso. These results will be published soon. I hope that the reseach publications will further help in getting funds from research grants.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : I am very happy for approving my project under TAS. In a very short time, the application is processed for providing the computational facilties. My sincere thanks to C-DAC, Pune.

Title of the work carried out: Quantum_Nano-PR

Name & Designation of the Chief Investigator: Dr. Jawar Singh, Prof. and Dean R &D.

E-mail Id:jawar@ iitp.ac.in

Institution Name: Indian Institute of Technology Patna, Bihta, Patna -801106 (Bihar).

Application Domain: Material Sciences and Computational Physics.

Research Challenge/s: According to the IRDs road map, the gate length of MOSFETs cannot be reduced beyond 12nm. This contradicts Denard's scaling theory that acts as a guideline to the semiconductor industry to miniaturize MOS technology in order to comply with Moore's Law. Thus it limits the usage of conventional materials in future device technologies. These issues motivated us to investigate 2D materials for future device applications like sensing, MOSFETs, spintronics, etc. because it is observed experimentally that 2D materials show far better electrostatics when compared to conventional 3D counterparts.

Work carried, Milestone, Achievements & Graphs, Plots:

We are using armchair silicene nanoribbons for caloritronics device application. One works on caloritronics applications will be communicated for review in the appropriate journal in the month of March 2022. PARAM Yuva II contributions will be acknowledged in my research in our communicated paper. We will be sharing graphs and plots in my work once they will get published.

Benefits & experience of using NPSF:

One work will be communicated in March 2022.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : The computational speed of the PARAM Yuva-II server is slow.

Title of the work carried out: Time Domain Free Vibration Simulation of Bridge Deck Sections

Name & Designation of the Chief Investigator: Dr Naresh K Chandiramani, Professor, department of Civil Engineering, IIT Bomabay Dr Abhijit Gogulapati, Assistant Professor, department of Aerospace Engineering, IIT Bombay

E-mail Id:kunal.ton@iitb.ac.in (user, other than CI)

Institution Name:IIT Bombay.

Application Domain: Computational Fluid Dynamics

Research Challenge/s: We wish to simulate free vibration response of a bridge deck section immersed in air flow. We wish to achieve this using overset mesh. For this we need OpenFOAM v1706. The current version of OpenFOAM available on the NPSF PARAM Yuva-II system does not meet our requirement.

Work carried, Milestone, Achievements & Graphs, Plots:

We did run some preliminary static CFD simulations using OpenFOAM software on the facility. We need to perform dynamic fluid structure interaction simulations, for which we need updated version of OpenFOAM v1706 with overset mesh solver overPimpleDyMfoam. We asked the CDAC help to update the OpenFOAM software to required version, but they were not able to update it because of incompatible hardware and compilers.

Benefits & experience of using NPSF:

As such we have only been able to carry out preliminary static CFD simulations using NPSF PARAM Yuva-II. For dynamic FSI simulations we have had to rely on our limited HPC resources at IITB, as the software version at NPSF PARAM Yuva-II does not meet our requirement.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work : Please try to update the software, hardware, and compilers present in the facility to meet our requirement.

Title of the work carried out: Electronic structure calculations of semiconductors

Name & Designation of the Chief Investigator: Dr. Subrata Deb, Assistant Professor (Stage-III)

E-mail Id:subrata.tu@gmail.com

Institution Name: Women's College (Affiliated to Tripura University)

Application Domain: Computational Physics/Material Science

Research Challenge/s: Density functional theory (DFT) or commonly known as first-principles

investigations providesaphenomenally successful approach to find the solutions of fundamental equations, that describesthe quantum behavior of atoms and molecules. This is extremely important to understand andcontrol the properties of matter at the level of individual atoms and molecules.Please specify about your research challenges faced while using the NPSF PARAM Yuva-II system for computation.

Work carried, Milestone, Achievements & Graphs, Plots:

A good number of computational works have been carried out using QE 6.5 for some known system (Ag, Fe, Al etc.) to get the initial idea about the computation works especifiallyscf calculation, energy gap calculation and band structure calculation.
It is relevant to mention here that I am working under the guidance of Dr. Sachin P Nanavati of University of Cardiff, United Kingdom and he is helping me a lot to understand the basic of this computational platform.

Benefits & experience of using NPSF:

I am in the beginning stage of the work. Presently doing some computations for known systems. Once the techniques of computations is understood then I shall be able to use this NPSF PARAM Yuva-II system for the quantum mechanical calculations of a good number of system as per the requirement of experimental physicists. As a preliminary user, I can say this platform really helpful for a beginner like me to work with this system. NPSF-PARAM system analyst is also very helpful and they used to help me as and when required from my end.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : Everything is fine about this system. But if it also tells about the rectification of errors (probable solution) then it would have been great for a new comer in this field.

Title of the work carried out: Photocatalytic reduction of Carbon dioxide (CO2) using Semiconductors

Name & Designation of the Chief Investigator: Dr Aman Kaura, Assistant Professor

E-mail Id:amankaura@pu.ac.in

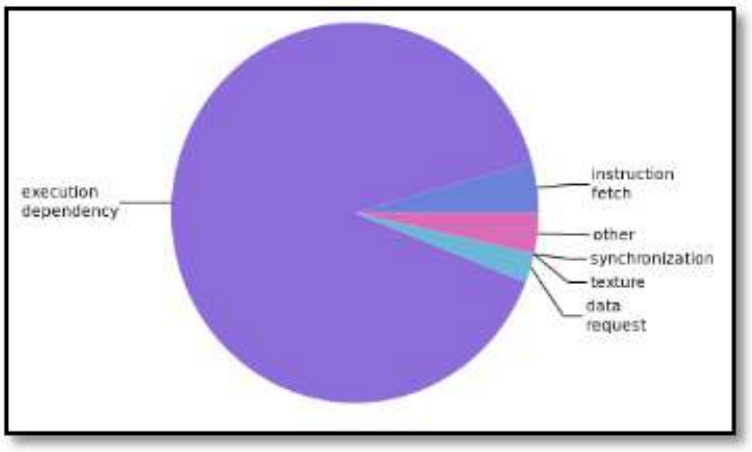
Institution Name: Panjab University Chandigarh

Application Domain: Chemical Sciences

Research Challenge/s: NIL

Work carried, Milestone, Achievements & Graphs, Plots:

Carbon nitride is increasingly used due to its extraordinary catalytic properties. It is successfully used in applications like CO2 reduction, photocatalytically hydrogen generation and photocatalytic breakdown of pollutants. However, pure Carbon nitride is characterized by very low photocatalytic efficiency due to high band gap and recombination of charges. Many strategies have been in use to overcome these limitations. With the help of dopants, we have improved the catalytic properties of carbon nitride. Theoretical simulations have been performed with the help of PARAM Supercomputing facility. The detailed work is under consideration of international journal. Results would be shared when the manuscript is accepted by the journal.



Stall reasons pie chart show high execution dependency, it is because of bandwidth constraints. These long dependencies are typically caused by dependencies on global memory. Pie chart was derived using NVIDIA Visual Profiler

Benefits & experience of using NPSF:

The work carried out has direct relevance to the society as it is related to minimize the impact of CO_2 in the atmosphere. I have acknowledged the National PARAM Supercomputing Facility (NPSF) of C-DAC, Pune, India for providing the cluster computing facility in the manuscript.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : CDAC Pune has provided the useful facility to the scientific community in India to carry out their research work

Title of the work carried out: Thermoelectric and topological Properties of novel mateirals

Name & Designation of the Chief Investigator: Aftab Alam, Associate Proessor

E-mail Id:aftab@iitb.ac.in

Institution Name: Department of Physics, IIT Bombay

Application Domain: Computational Physics

Research Challenge/s: Large scale simulation was not possible to run. Small scale simulation was done successfully.

Work carried, Milestone, Achievements & Graphs, Plots:

We are working on fundamental science aspect of renewable energy materials in collaboration with experimentalists.

Benefits & experience of using NPSF:

It helped to performs few intial level calculations.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : We appreciate your comments/feedback/suggestions to improve our system

Work Report 24 Summary

Title of the work carried out: Simulation of Atmospheric turbulence over land

Name & Designation of the Chief Investigator: Prof. Abhijit Gogulapati

E-mail Id:203010044@iitb.ac.in

Institution Name: IIT Bombay

Application Domain: Climate and Environmental Sciences

Research Challenge/s: Perform a grid convergence study, forecasting various atmospheric profiles in the time scale of 4hr – 24hrs

Work carried, Milestone, Achievements & Graphs, Plots:

We performed Large Eddy simulations of Atmospheric Boundary Layer using an open source code called Meso-NH. Our objective is to forecast the profiles of Temperature, wind velocity for a 24hr cycle. Achievements – We were able to simulate day time evolution (i.e. from 6a.m – 6p.m) of the near surface atmosphere in dry conditions.

Benefits & experience of using NPSF:

The cluster allowed us to efficiently utilize the parallel capabilities of the code for performing very long studies on evolution of the atmosphere.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : The costumer service provided by the system admins is commendable.

Title of the work carried out: Molecular Dynamic Simulation of Biological Macromolecules

Name & Designation of the Chief Investigator: Prof. Shahid M. Nayeem

E-mail Id:msnayeem.ch@amu.ac.in

Institution Name: Aligarh Muslim University

Application Domain: Bio Sciences/ Bioinformatics

Research Challenge/s: (a) Understanding protein aggregation and folding (b) Drug protein interaction

Work carried, Milestone, Achievements & Graphs, Plots:

Published following four papers where NPSF-PARAM YUVA Facility is mentioned in Acknowledgement.

1. Jahan, I.; Nayeem, S. M., Destabilization of Alzheimer's Aβ42 protofibrils with acyclovir, carmustine, curcumin, and tetracycline: insights from molecular dynamics simulations. New Journal of Chemistry 2021, 45, (45), 21031-21048.
2. Mustafa M., Ali A, Siddiqui S.A., Mir A.R., Kausar T.,Nayeem S.M., Minhal Abidi & Safia Habib, Biophysical characterization of structural and conformational changes in methylmethane sulfonate modified DNA leading to the frizzled backbone structure and strand breaks in DNA. J. Biol. Structure and Dynamics. https://doi.org/10.1080/07391102.2021.1899051.
3. Siddiqui, S., Ameen, F., Kausar, T., Nayeem S.M., Rehman S.U., Tabish, M., Biophysical insight into the binding mechanism of doxofylline to bovine serum albumin: An in vitro and in silico approach. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 249 (2021) 119296.
4. Ameen, F., Siddiqui, S., Jahan I., Nayeem S.M., Rehman S.U., Tabish, M., Studying the interaction of scopolamine with calf-thymus DNA: An in-vitro and in-silico approach and genotoxicity. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 265(2022) 120391.

Copy of these papers are attached for the graphs and plots etc.

Benefits & experience of using NPSF:

MD simulation of large biological macromolecules using GROMACS version 5.1.2 are carried out on the NPSF PARAM Yuva-II system.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : If possible please enhance the 120 hours restriction of simulation to 240 hours

Title of the work carried out: Atomistic Modelling of Nanomaterials for Mechanical Characterization.

Name & Designation of the Chief Investigator: Dr Rajesh Kumar

E-mail Id:rpawar@nith.ac.in

Institution Name:NIT Hamirpur

Application Domain: Computational Materials Science

Research Challenge/s: We are working on exploring the mechanical behaviour of graphene and h-BN based nanomaterials and their metal matrix based nanocomposites.

Work carried, Milestone, Achievements & Graphs, Plots:

Work is under progress. We have done few simulations for mechanical behaviour of graphene/h-BN based lateral heterostructures.

Benefits & experience of using NPSF:

We need multicores to run our parallel programs and PARAM Yuva-II has provided us that platform to succeed in our aim.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : Support system could be better. Sometimes we don't get any response to our queries.

Title of the work carried out: Aerosol Radiative forcing over India (ARFI) and Atmospheric Trace Gases, Chemistry, Transport and Modelling (AT-CTM)

Name & Designation of the Chief Investigator: Dr. Binita Pathak, Assistant Professor of Department of Physics, Dibrugarh University

E-mail Id:rs_arshinisaikia@dibru.ac.in

Institution Name: Department of Physics & Centre for Atmospheric Studies, Dibrugarh University

Application Domain: Climate & Environment Sciences

Research Challenge/s: The biggest challenge we faced was to remain in a long queue to get the job done.

Work carried, Milestone, Achievements & Graphs, Plots:

The NPSF PARAM Yuva-II system provides us the computational support with the help of which we can address or answer the scientific questions related to climate change and natural hazards such as lightning and their impacts over the Eastern Himalayas foothills regions.

Benefits & experience of using NPSF:

NPSF PARAM Yuva-II system gives the platform to simulate and get the outputs from computationally expensive models such as WRF-Chem, which we cannot run on a normal computer. Moreover, upon request, they also provide us the memory space to store large datasets for a specific time. And technical support is all time available whenever we get stuck.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : We are thankful and highly appreciate it if NPSF PARAM Yuva-II reduces the job queue time for our future research.

Work Report 28 Summary

Title of the work carried out: Computational studies on β1 adrenergic receptor

Name & Designation of the Chief Investigator: Dr. Manali Joshi, Assistant Professor, S. P. Pune University

E-mail Id:manalijoshi@unipune.ac.in

Institution Name: Bioinformatics Centre, S. P. Pune University

Application Domain: Bioinformatics

Research Challenge/s: None

Work carried, Milestone, Achievements & Graphs, Plots:

Manuscript is being written.

Benefits & experience of using NPSF:

The account on NPSF PARAM Yuva-II enabled running microsecond timescale protein simulations.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work : None.

Title of the work carried out: Electronic and thermoelectric behavior of 2D KCuSe.

Name & Designation of the Chief Investigator: Dr.Soumya Jyoti Ray , Assistant Professor, IIT Patna

E-mail Id:ray@iitp.ac.in

Institution Name: Indian Institute of Technology Patna

E-mail Id: ray@iitp.ac.in

Institution Name: Indian Institute of Technology Patna

Application Domain: Computational Physics

Research Challenge/s: Our project work is mainly based on Density Functional Theory (DFT) calculations. Some of the calculations are computationally expensive and also time consuming.

Work carried, Milestone, Achievements & Graphs, Plots:

We have investigated the phononic, electronic and thermoelectric properties of 2D KCuSe. The thermoelectric properties mainly include the electrical conductivity, seebeck coefficient, thermoelectric power and figure of merit(zT) at different temperatures.

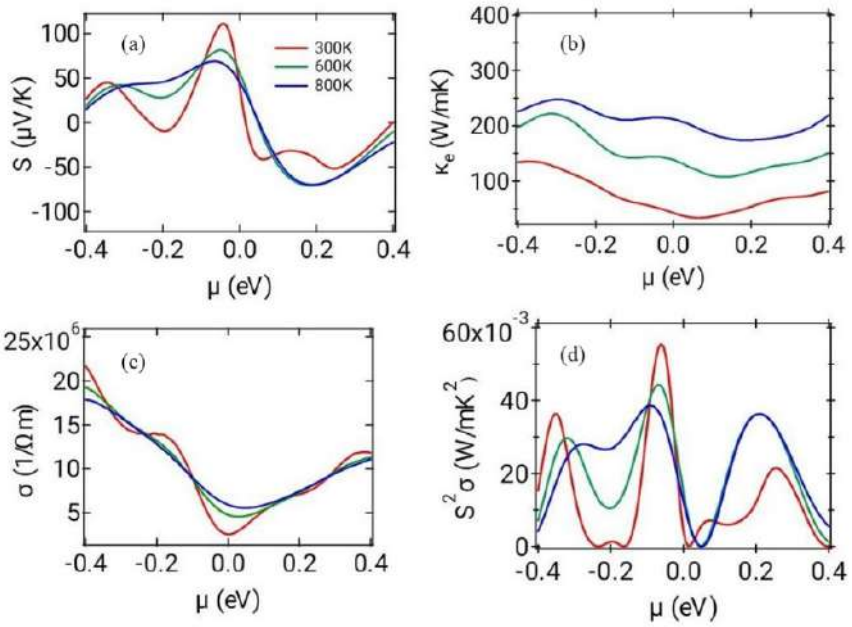


Fig: (a) Seebeck coefficient, (b) thermal conductivity, (c) electrical conductivity, and (d) power factor for 2D KCuSe.

Benefits & experience of using NPSF:

The PARAM Yuva II facility was very much useful and robust. The maintenance of job queues was also comfortable. Therefore, we can get a opportunity to run more complex and computationally demanding calculations.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : Nodoubt, CDAC , Pune has been doing good job in computational field but I personally found the help desk was not very much supportive.

Title of the work carried out: Computational insights into the inhibitory mechanism of peptide inhibitors against amyloid- βaggregation and protofibril destabilization

Name & Designation of the Chief Investigator: Dr. Deepti Goyal (Ph.D.), Assistant Professor

E-mail Id:deeptig@iitbombay.org

Institution Name: Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab.

Application Domain: Bioorganic and Computational Chemistry

Research Challenge/s:

To elucidate the binding interactions of peptide inhibitors with Aβ peptide using molecular dynamics. To understand the inhibition mechanism of peptide inhibitors towards Aβ peptide aggregation and disaggregation by computational methods

Work carried, Milestone, Achievements & Graphs, Plots:

Amyloid deposits have emerged as a key player in the pathogenesis of Alzheimer's disease (AD). According to clinical studies, the development of Alzheimer's disease (AD) is linked to the abnormal aggregation of amyloid–β (Aβ) peptide into toxic fibrillar deposits. The most acceptable therapeutic strategies for the treatment of AD is to inhibit the production of β–sheet rich structures. Liu et al. reported a decapeptide, D–enantiomeric RTHLVFFARK–NH2 (rk10), which acts as a potent inhibitor against amyloid–β protein aggregation. The binding sites of rk10 with Aβ42 monomer and protofibril have been identified using molecular docking studies in the present work, which demonstrated that rk10 displayed –5.3 kcal/mol binding affinity with Aβ42 monomer and –6.9 kcal/mol with Aβ42 protofibril (Figure 1). Further, molecular dynamics (MD) simulations have been performed to elucidate the inhibitory mechanism of rk10 against Aβ42 aggregation and disaggregation. The MD simulations indicated that rk10 showed discrete binding abilities with residues across N– to C– terminal including central hydrophobic core (CHC) region of Aβ42 monomer as well as Aβ42 protofibril and restricts the conformational changes of α–helix structure of Aβ42 into another secondary structure content such as β–sheet, coil, and turn. These results are correlated well with NMR and CD spectra of Aβ42 monomer + rk10. RMSD and RMSF results highlighted the stabilization of Aβ42 monomer and destabilization of Aβ42 protofibril in the presence of rk10. Hydrogen bonding and π–π interaction contributed to the strong binding of rk10 with Aβ42 monomer as well as Aβ42 protofibril. The per–residue binding free energy analysis highlighted that Glu3, Asp7, Glu11, His14, Gln15, Leu17–Phe19, Glu22, Asp23, Gly37, and Ala42 residues of Aβ42 are responsible for favorable binding free energy of rk10 with Aβ42 monomer and protofibril. The binding free energy (MM–PBSA) analysis highlighted that non–bonded van der Waals interactions, electrostatic interactions, and non–polar solvation energy are the governing force involved in the binding of rk10 with Aβ42 protofibril. MD simulations revealed that rk10 reduced Aβ42 aggregation by restricting Aβ42 monomers to a helical shape and destabilizing the Aβ42 protofibril structure. Overall, the present study elucidates how rk10 inhibited the Aβ42 aggregation process, which would be beneficial in the structure–based drug design of potent antagonist against Aβ42 aggregation and disaggregation to control the progression of AD.

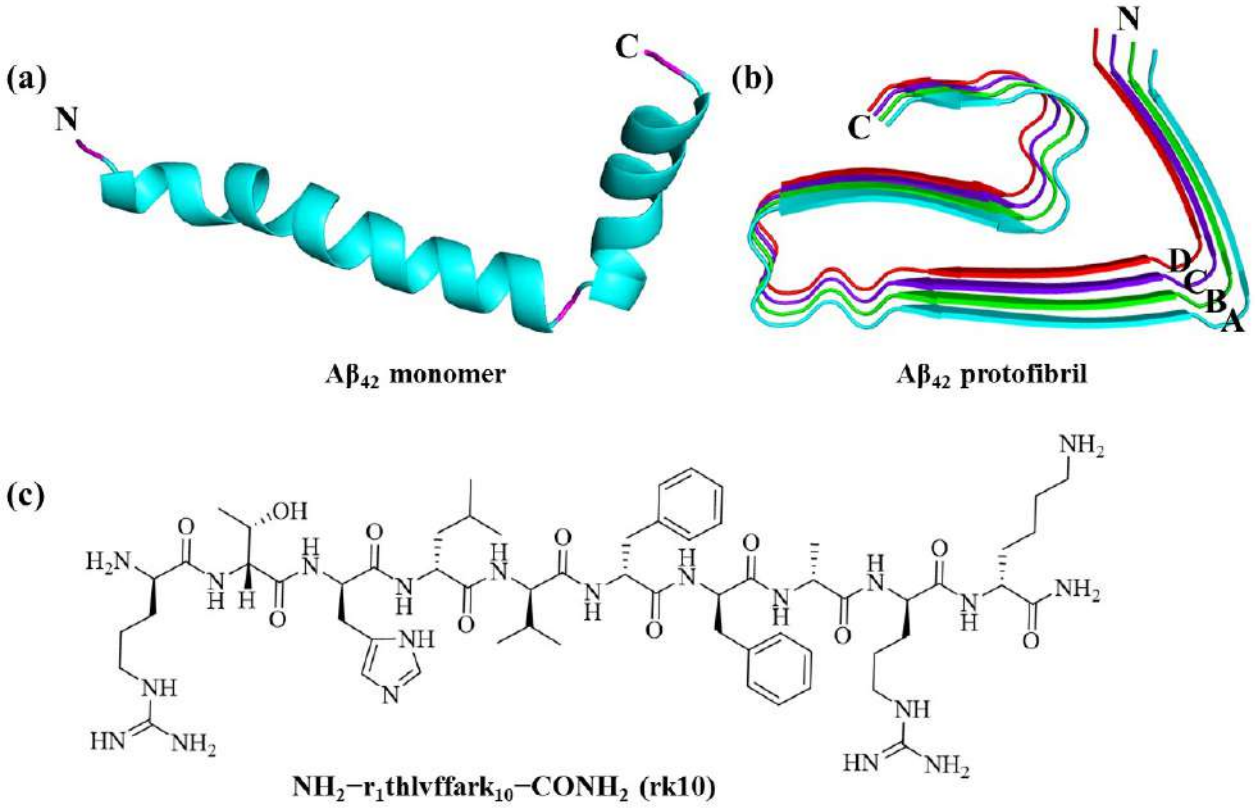


Figure 1: The cartoon representation of the native structure of Aβ42 monomer (PDB ID: 1IYT) and Aβ42 protofibril (PDB ID: 5OQV) with labelled N– and C– termini are shown in panel a, and b, respectively. The 2D chemical structure of rk10 is shown in panel c.

The abnormal self–assembly of β–amyloid (Aβ) peptide plays a key role in the pathogenesis of Alzheimer's disease (AD). The other factors such as the dys–homeostasis of biometals (Cu2+, Fe2+, Zn2+), oxidative stress and cellular toxicity also involves in the pathology of AD. Due to the lack of knowledge behind the molecular mechanism of AD, there is no such potential drug until a date that can completely cure or halt the progression of disease. So, there is an urgent need for new therapeutic drugs of AD with different mechanisms of action. In this regard, Pradhan and coworkers reported a multifunctional peptoid inhibitor 1AIIAL5 (AI) against AD possessing high selectivity, stability and bioavailability. To get insight into the inhibitory mechanism of AI peptoid against Aβ1–42 monomer at atomic level, in this work we carried out the molecular docking and classical molecular dynamic (MD) simulations. Molecular docking revealed favorable binding of AI peptoid with Aβ1–42 monomer (Figure 2). Further, MD results indicated the stabilization of Aβ1–42 monomer in presence of AI peptoid. Decreased RMSD, Rg, RMSF and SASA values clearly indicates the stabilization of Aβ1–42 monomer in presence of AI peptoid. In addition, significant enhancement in helical content, diminution in β–sheet content and disruption of salt bridge highlighted the conservation of non–aggregation state of Aβ1–42 monomer. The experimental study like CD spectra and Thioflavin T assay also indicated the no β–sheet formation and inhibition of Aβ1–42 aggregation in the presence of AI–peptoid. The binding free energy analysis by molecular mechanics Poisson–Boltzmann surface area (MM–PBSA) method suggested that AI peptoid interacts with the N–terminal, CHC region and C–terminal region of Aβ1–42 monomer thereby inhibited the conformational transition of Aβ1–42 monomer into the aggregation prone structure. This work will provide valuable information for the invention of effective drug candidates to halt Aβ aggregation.

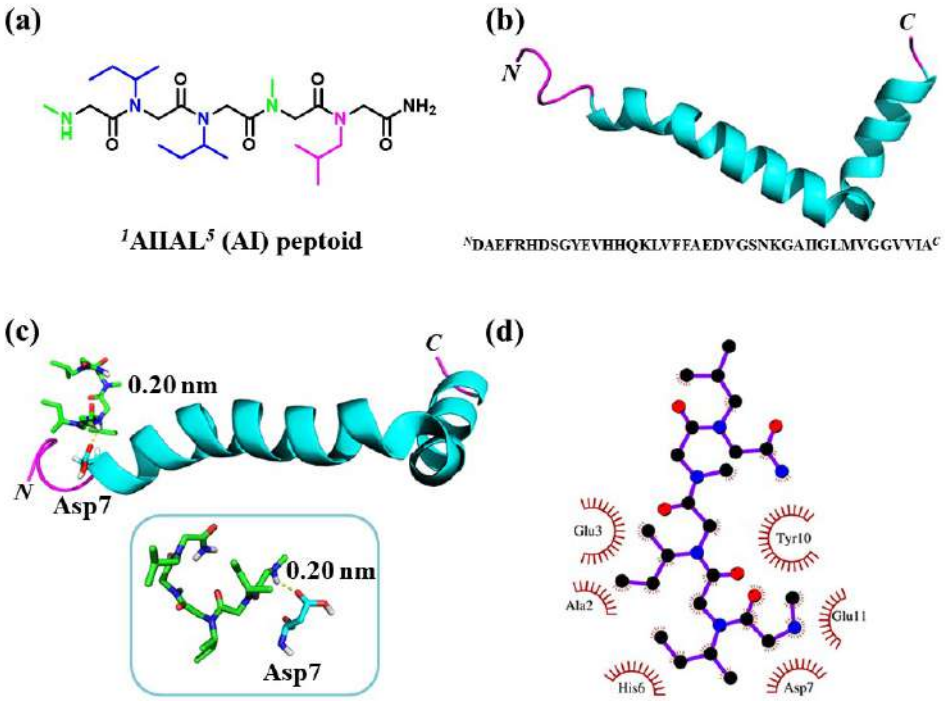


Figure 2: The chemical structure of AI peptoid is shown in panel a. The Aβ1–42 monomer (1IYT) is shown in the cartoon representation with N– and C– termini labelled in panel b. The docked complex of AI peptoid with Aβ1–42 monomer (PDB ID: 1IYT) highlighting the best–docked conformation is shown in panel c. The Aβ1–42 monomer structure is shown in the cartoon representation and AI peptoid is shown in the stick representation. H–bond is represented as yellow dashed line. The 2D interaction map displaying hydrophobic contacts of Aβ1–42 monomer with AI peptoid is shown in panel d. The Aβ1–42 residues involved in hydrophobic contacts are shown in red semicircles. The maps were generated using LigPlot+ software.

Benefits & experience of using NPSF:

The computational facility provided by CDAC is of great support to the Ph.D. and M.Sc. students to pursue their research projects and timely completion of research work. In the 2020–2021 pandemic years, the facility of CDAC gave a great opportunity to students to continue their research work. The benefit of the NPSF is that the simulations can be completed in short time and students could set up the simulations easily. The staff at CDAC is very cooperative and quickly responded to our queries. We are very much thankful and obliged to be a part of this wonderful NPSF family.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work : None.

Title of the work carried out: Oxide Ion Transport in ZrO2 based Solid Electrolyte of SOFC using Molecular Dynamics simulation

Name & Designation of the Chief Investigator: Prof. Padma Kumar Padmanabhan

E-mail Id: Madhual@iitg.ac.in

Institution Name: Indian Institute Of Technology–Guwahati

Application Domain: Computational Physics/ Material Sciences

Research Challenge/s: None

Work carried, Milestone, Achievements & Graphs, Plots:

Manuscript is being written.

Benefits & experience of using NPSF:

Tools like LAMMPS, QUANTUM ESPRESSO, PLUMED, CPMD, CP2K built-in NPSF PARAM Yuva-II are used for simulation, and compiler intel fortran, C++ are also used for analysis purposes.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work : None.

Title of the work carried out: Study of Heusler alloys for spintronics and thermoelectric applications

Name & Designation of the Chief Investigator: Prof. Atul Saxena, Professor

E-mail Id:asaxena@nehu.ac.in , DIPANGKAR@nehu.ac.in

Institution Name: North-Eastern Hill University

Application Domain: Computational Physics

Research Challenge/s: The main challenge that we faced was the "PORT" issue. The NPSF uses port 22 and our University blocks port 22 for security reasons. Solving this simple issue alone took months.

Work carried, Milestone, Achievements & Graphs, Plots:

We used the preinstalled Quantum ESPRESSO package. But its quite surprising that the NPFS is still offering its 5.1 version which is capable of doing very basic DFT calculations, while 7.1 version is already available.

Benefits & experience of using NPSF:

As mentioned earlier, we are still facing the port issue, and being the outdated version of the Quantum ESPRESSO, the use of NPSF didn't benefit us much.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work :
I will strongly suggest updating the software and codes, especially the ones which are available in open source.

Title of the work carried out: Novel perovskite-based solar cells: Investigation of potential properties using ab-initio approaches

Name & Designation of the Chief Investigator: Dr. Yogesh Sonvane Assistant Professor at Sardar Vallabhbhai National Institute of Technology

E-mail Id:yas@phy.svnit.ac.in

Institution Name: Sardar Vallabhbhai National Institute of Technology.

Application Domain: Material Science / Computational Physics

Research Challenge/s: We need high computational powers to simulate large material systems.

Work carried, Milestone, Achievements & Graphs, Plots:

We have used NPSF PARAM Yuva-II to complete our Density Functional Theory calculations for studying perovskite materials.

Benefits & experience of using NPSF:

Due to the excellent capacity of your system, we have utilized it to calculate many properties like optical, thermal, vibrational, and mechanical, and it also made our work easier.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work :

We appreciate your comments/feedback/suggestions to improve our system.

Title of the work carried out: Atomistic Computer Simulation of Fast Ion Conducting Solids

Name & Designation of the Chief Investigator: Prof. Padma Kumar Padmanabhan / Professor

E-mail Id:padmakumarp@iitg.ac.in

Institution Name: Indian Institute Of Technology Guwahati, Guwahati, Assam.

Application Domain: Computational Physics/ Material Sciences

Research Challenge/s: Charges waived off by C-DAC due unavailability funds.

Work carried, Milestone, Achievements & Graphs, Plots:

Submitted a manuscript titled "Understanding Oxide Ion Transport In Yttria Stabilized Zirconia: Molecular Dynamics Investigation", co-authored by Ms. S. Madhual and Dr. K. Pramanik. The work duly acknowledge the generous computational time allotted to the group.

Benefits & experience of using NPSF:

Non-commercial (under GPL) softwares such as LAMMPS, QUANTUM ESPRESSO, PLUMED, CPMD, CP2K installed in NPSF PARAM Yuva-II are used for simulation, and compilers intel fortran, C++ are also used for development and data analysis purposes.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF PARAM Yuva-II for your research work :
Well, we are facing some issues with the presently installed version of LAMMPS, QUANTUM ESPRESSO in interfacing with PLUMED. Our attempts to install the right versions compatible with PLUMMED, within the group's space/permissions, were also not quite successful. Kindly, offer the users better (interactive, if possible!) help with the installation of non-commercial software (under General Public License).

Title of the work carried out: Study of thermoelectric properties of bulk nanostructured materials using Monte Carlo Simulations.

Name & Designation of the Chief Investigator: Dr. Neeleshwar Sonnathi (Assistant Professor, USBAS, GGSIP University) CI (Chief Investigator)
Dr Anjana Bagga (Assistant Professor, USBAS, GGSIP University) Co-CI (Collaborator)

E-mail Id:sn@ipu.ac.in

Institution Name: Guru Gobind Singh Indraprastha University, New Delhi 110078.

Application Domain: Material Sciences

Research Challenge/s: We still have to harness the full potential of the current state of art computational power given to us for some heavy computational work load which is kept for the future research tasks. For now, we are satisfied with the current computational facility.

Work carried, Milestone, Achievements & Graphs, Plots:

Paper published using this NPSF PARAM Yuva II systems

Name of the Journal; Nanotechnology

Impact Factor; 3.399

Srikanth Mandava, Neeta Bisht, Anjali Saini, Mukesh Kumar Bairwa, Khasimsaheb Bayikadi, Ankita Katre and Neeleshwar Sonnathi, "Investigating the key role of carrier transport mechanism in SnSe nanoflakes with enhanced thermoelectric power factor, Nanotechnology (2021).

Benefits & experience of using NPSF:

Using the NPSF PARAM Yuva-II system we were able to conduct our research work smoothly and we published one journal article using the above facility.

Any comments/feedback/suggestions in terms of your exclusive experience on NPSF

PARAM Yuva-II for your research work : Publication: Sivakumar V., Ankit. G., Biju C., (2021), Geospatial Information Extraction from Big Satellite Data using CUDA-enabled GPU Parallel Computing Technique, Journal of Geomatics, 15 (2), 152-159.

7.3 Appendix 'C' Users across Institutions

Below is the list of NPSF PARAM Yuva-II users across institutions.

Table : NPSF PARAM Yuva-II users across academic institutions

State	Academic Institutes	No. of Users
Assam	Assam University, Silchar	1
	Dibrugarh University, Dibrugarh	3
	Indian Institute of Technology (IIT), Guwahati	30
	National Institute of Technology (NIT), Silchar	3
Bihar	Central University of South Bihar (CUSB), Patna	1
	Indian Institute of Technology (IIT), Patna	12
Chandigarh	Panjab University , Chandigarh	16
Delhi	Guru Gobind Singh Indraprastha University, Delhi	4
	Indian Institute of Technology (IIT), Dehli	8
	Indraprastha Institute of information technology, Delhi	4
	Jamia Millia Islamia University, New Delhi	7
	Jawaharlal Nehru University (JNU), Delhi	2
	University of Delhi, New Delhi	4
Goa	Goa University	2
Gujarat	Ahmedabad University,Ahmedabad	2
	Central University of Gujarat (CUG), Gandhinagar	3
	Government Engineering College, Modasa	1
	Indian Institute of Technology (IIT), Gandhi Nagar	10
	SVNIT , Surat	14
	St. Xaviers College, Ahmedabad	1
Haryana	Central University of Haryana (CUH), Jant-Pali	4
	Guru Jambheshwar University of Science and Technology Hisar	2
	Kurukshetra University, Kurukshetra	5
Himachal Pradesh	Central University of Himchal Pradesh, Shahpur	2
	Himachal Pradesh University , Shimla	7
	National Institute of Technology, Hamirpur	2
Jammu and Kashmir	University of Kashmir, Srinagar	2
Jharkhand	Indian Institute of Technology (Indian school of Mines),Dhanbad	7
Karnataka	Indian Institute of Astrophysics, Bengaluru	12
	Indian Institute of Science (IISC), Bengaluru	7
	LGC Promochem India Pvt Ltd, Bengaluru	1
	Maharani's Science College for Women, Bengaluru	1
	Manipal University, Bengaluru	2
	University of Mysore, mysore	2

Table : NPSF users across academic institutions

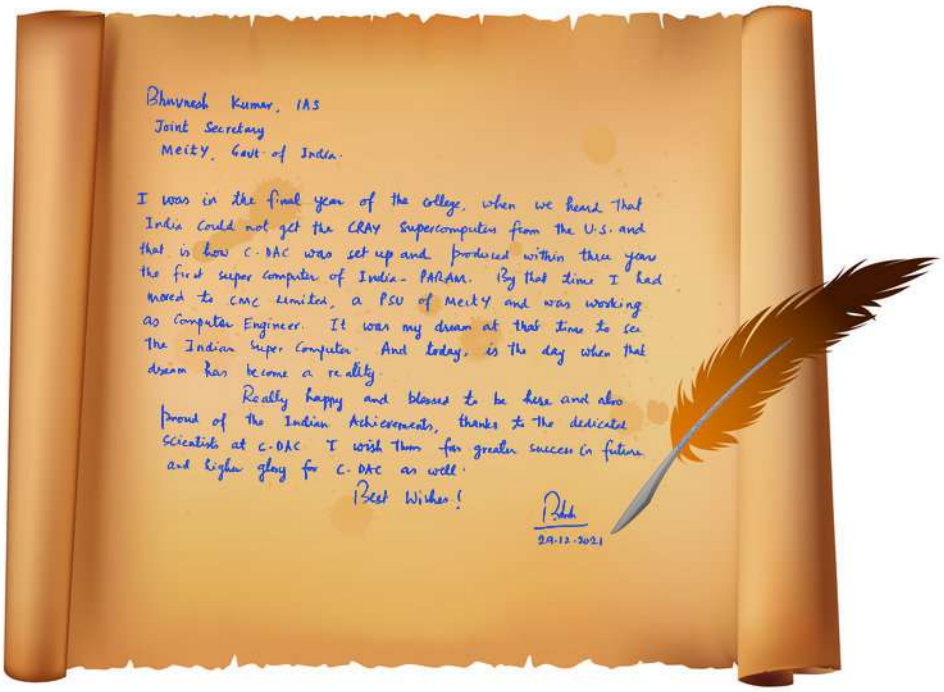
State	Academic Institutes	No. of Users
Kerala	IISER, Thiruvananthapuram	3
	IIST, Thiruvananthapuram	2
	IIIT Kottayam	7
	National Institute of Technology (NIT), Calicut	1
Madhya Pradesh	(ABV- IIITM), Gwalior	6
	Jiwaji University, Gwalior	3
Maharashtra	Ahmednagar College, Ahmednagar	1
	Army Institute of Technology(AIT), Pune	5
	Bhusawal Arts, Science and PO Nahata Commerce College, Jalgaon	1
	College of Engineering (COEP), Pune	8
	D Y Patil University,Pune	3
	H.P.T Arts and R.Y.K. Science College, Nasik	3
	IISER, Pune	68
	IIT, Bombay	277
	JSPM TSSM College, Pune	1
	Maharashtra Institute of Technology, Pune	1
	PVPIT, Pune	3
	RTMNU , Nagpur	2
	Savitribai Phule Pune University, Pune	43
	Shivaji University, Kolhapur	2
	SRTMUN , Nanded	2
	Symbiosis Institute of Technology (SIT), Pune	1
	Tetrahydrix Engg. Pvt. Ltd. (TEPL), Pune	1
	VNIT , Nagpur.	10
	Whistling Woods International Institute (WWII), Mumbai	2
Meghalaya	North-Eastern Hill University, Shillong	3
Mizoram	Pachhunga University College , Aizawl	1
Odisha	Indian Institute of Technology (IIT), Bhubaneswar	7
	IISER, Berhampur	4
	Kalinga Institute of Industrial Technology (kiit), Bhubaneswar	2
	National Institute of Technology Rourkela (nitrkl)	1
Pondicherry	Pondicherry University, Pondicherry	5

Table : NPSF users across academic institutions

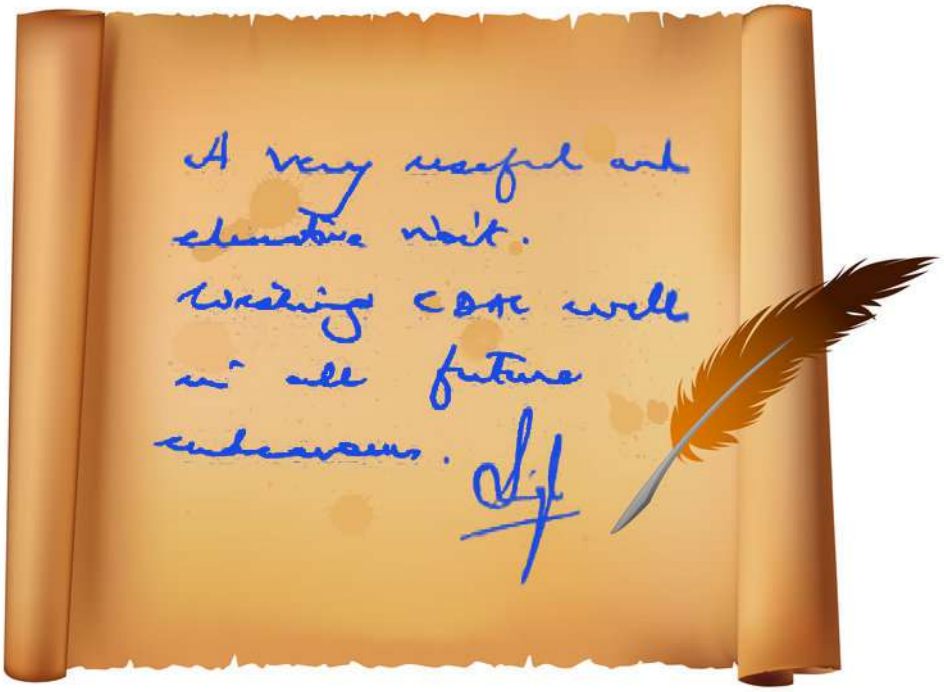
State	Academic Institutes	No. of Users
Punjab	Dr. B R Ambedkar National Institute of Technology, Jalandhar	1
	Guru Nanak Dev University, Amritsar	1
	IISER, Mohali	1
	Indian Institute of Technology (IIT),Ropar	11
	Institute of Nano Science and Technology (INST), Mohali	25
	Sri Guru Granth Sahib World University,Fatehgarh Sahib	11
Rajasthan	Cetral University of Rajsthan (CURAJ), Ajmer	1
	Government College, Tonk	1
	Gramin Mahila P.G. College , Sikar, Rajasthan	1
	Indian Institute of Technology (IIT), Jodhpur	14
	Pandit Deendayal Upadhyaya Shekhawati University, Sikar	1
	University of Rajastan, Jaipur	1
Tamil Nadu	Anna University, Chennai	2
	Periyar University,Salem	2
	SASTRA, Thanjavur	3
	University of Madras, Chennai	1
	SRM Institute of Science and Technology,Kattankulathur	6
Tripura	Women's College, Agartala	1
Uttar Pradesh	Aligarh Muslim University (AMU), Aligarh	7
	Amity University, Noida	2
	Banaras Hindu University, Varanasi	4
	Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur	1
	Galgotias University, Greater Noida	1
	GLA University, Mathura	1
	J.C. Bose University of Science and Technology, YMCA,Faridabad	1
	Indian Institute of Technology (IIT), Kanpur	31
Uttarakhand	Indian Institute of Technology (IIT), Roorkee	5
West Bengal	Indian Institute of Engineering Science and Technology, Shibpur	1
	Indian Institute of Science Education and Research (IISER), Kolkata	2
	Indian Institute of Technology (IIT), Kharagpur	13
	Total	867

7.4 Appendix 'D' Quotes by Dignitaries & Visitors

Visitors Quotes

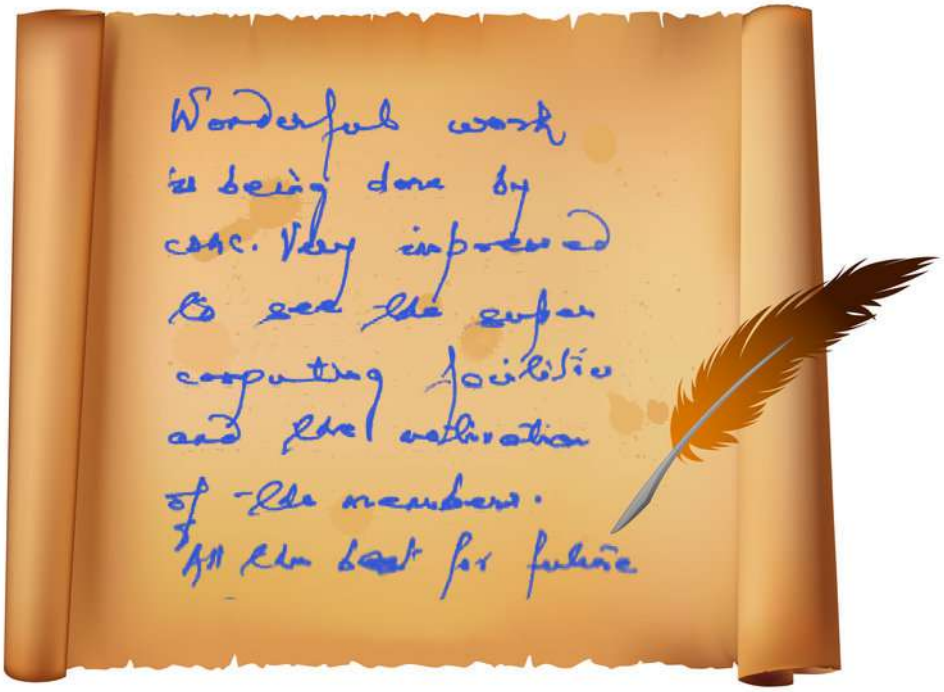


Buvnesh Kumar,IAS, Joint Secretary, Meity,Govt.of India.

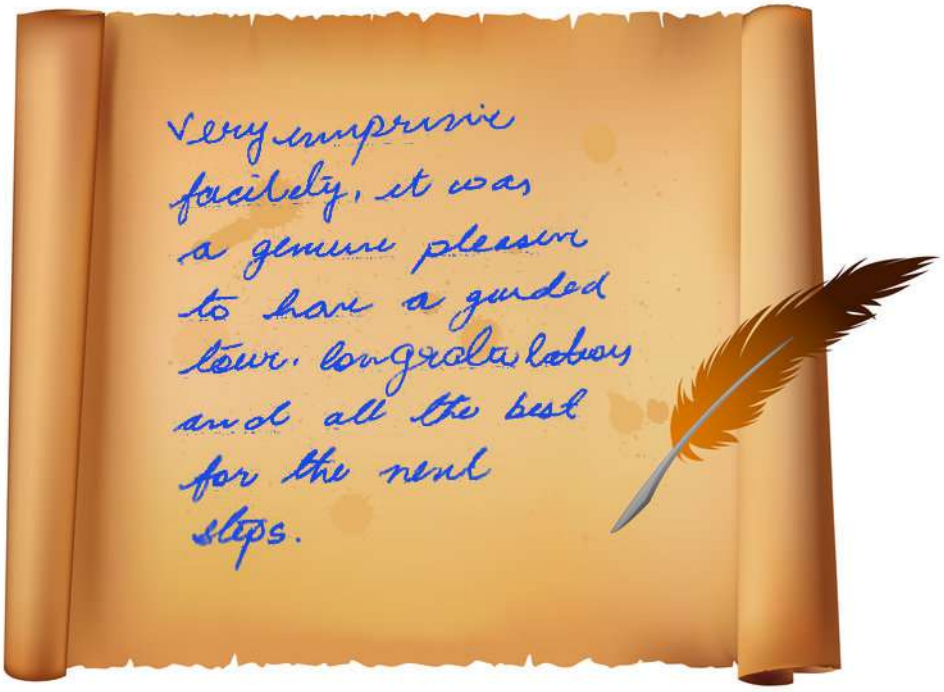


Lt.Gen Ranbir Singh(Retd)

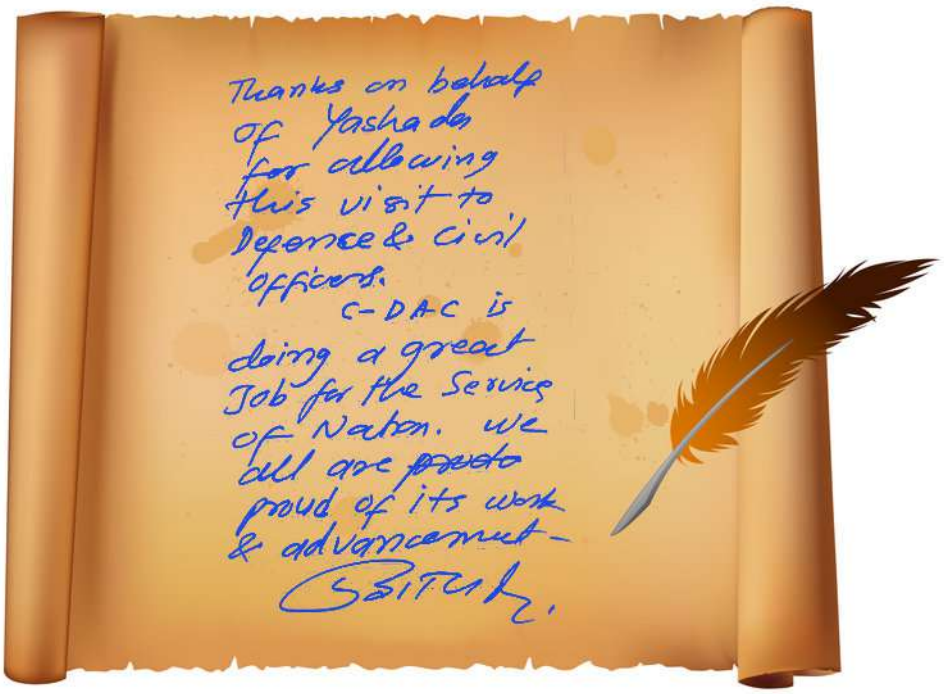
Lokender Singh,IPS, Haryana Cadre



Lt Colonel S Panda

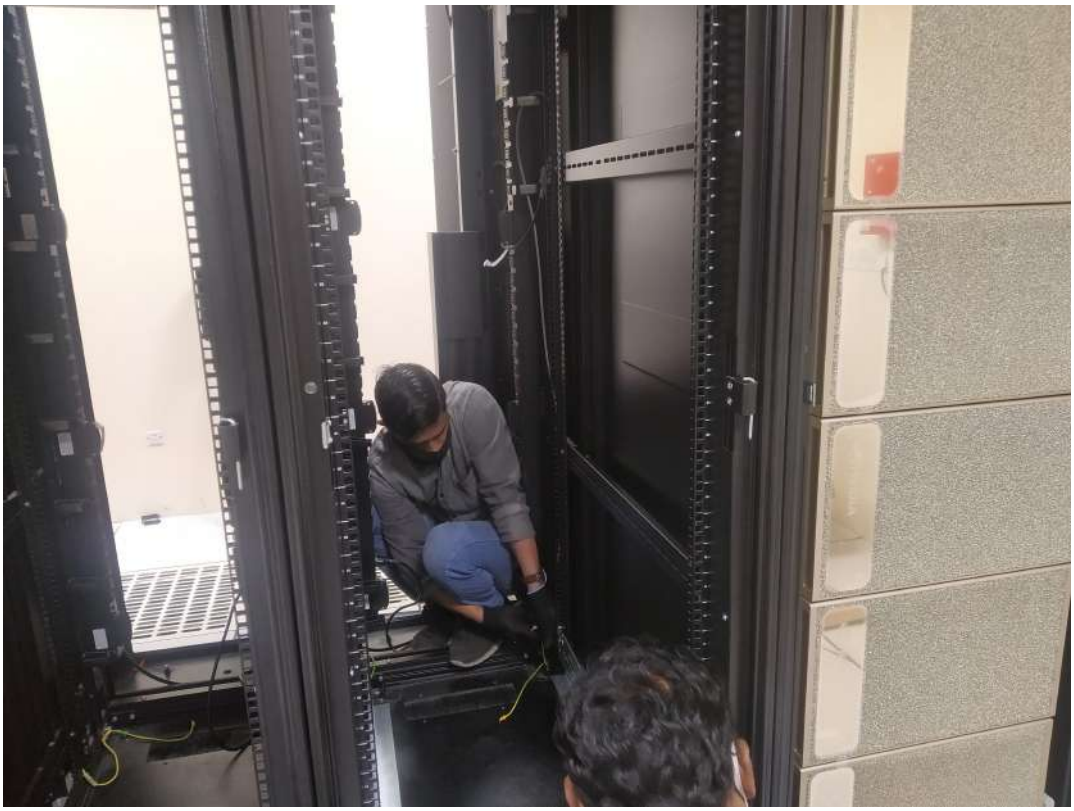


Jayaram Chengulur,Distinguished Professor, NCRA-TIFR, Pune



Prakas Pote, Additional Director, YASHADA, Pune

7.5 Appendix 'E' Picture Gallery



PARAM Siddhi-AI System Commissioning at NPSF, CIP.

PARAM Siddhi-AI System Commissioning at NPSF, CIP.

PARAM Siddhi-AI System Commissioning at NPSF, CIP.

PARAM Siddhi-AI System Commissioning at NPSF, CIP.

PARAM Siddhi-AI System Commissioning at NPSF, CIP.

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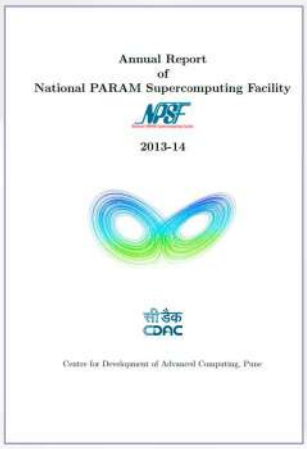

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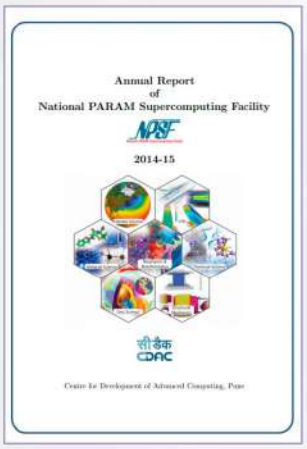

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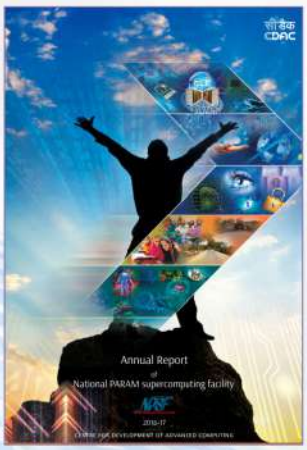

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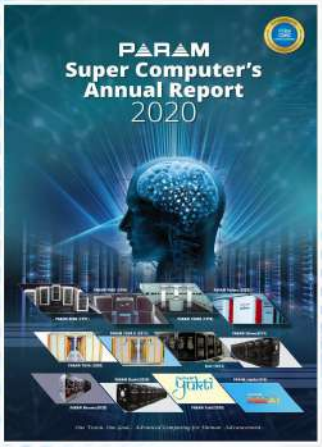
2019



2020

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