National PARAM Supercomputing Facility

Annual Report 2020

One Vision. One Goal... Advanced Computing for Human Advancement...

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Cover Note

Dear Reader,

We feel proud to present PARAM Supercomputing Facilities Annual Report for the year 2020. The information in the report provides both qualitative and quantitative indices of work carried out using PARAM Supercomputing Facilities, 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 the qualitative part, more especially 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 the report attached, for which you may write to npsf-report@cdac.in e-mail address.

Happy Computing!

Regards
NPSF

आवरण पत्र

प्रिय पाठक गण,

हम परम सुपरकंप्यूटिंग सुविधाओं की वर्ष 2020 की वार्षिक रिपोर्ट प्रस्तुत करते हुए गौरवान्वित महसूस कर रहे 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-report@cdac.in पर ईमेल कर सकते हैं।

शुभ कंप्यूटिंग, सशक्त कंप्यूटिंग!

भवदीय,

एनपीएसएफ

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Dr. Hemant Darbari
Director General, C-DAC

Message from Director General

I am proud to place this exclusive report on usage statistics and activities carried out on PARAM Supercomputing Facilities for the year 2020-21.

C-DAC has done pioneering work both in HPC and AI for the last three decades. With the enhanced compute capabilities, the application of AI in various thrust areas like Video Analytics, Brain Computing, NLP and Speech Technologies, Robotics etc. has drastically increased.

Year 2020 was announced as "HPC-AI Convergence Year". With the successful implementation of PARAM Siddhi-AI, the first and fastest 210 AI Petaflop Scalable Supercomputer, C-DAC raised the curtain for HPC-AI Convergence.

My memories go way back to the Year 2013, a major milestone in the history of NPSF. The launch of PARAM Yuva II, 1st Hybrid and Power-efficient System in the country ranked in both the Top 500 and Green 500 Computers of the world. Since then, NPSF has been the trendsetter among the World's leading HPC Systems, achieved record utilization and uptime of the system over and above 90%. For all the successive years from 2013, each year NPSF saw the ever-increasing demand for the HPC resources with a record execution of 4.75 Lac HPC jobs across 350 Projects, 1200+ users from 130+ Organizations.

These encouragement figures over the years helped in culminating the idea of having multiple and many fold HPC facilitates in the country through National Super Computing Mission (NSM). Under NSM, C-DAC successfully deployed PARAM series of Supercomputers, the first being PARAM-Shivay with a peak performance of 837 Tera Flops at IIT BHU, Varanasi, PARAM Shakti with a peak performance of 1.66 Peta Flops at IIT, Kharagpur and PARAM-Brahma with peak performance of 800 Tera Flops at IISER Pune and PARAM Yukti with peak performance of 833 Tera Flops at JNCASR. The launch of PARAM Shivay and PARAM Brahma by our honorable Prime Minister Shri. Narendra Modiji speaks out the importance of this Mission and the commitment of C-DAC toward Research initiatives in the country. The systems have executed more than 15 Lac HPC jobs till now.

The Bioinformatics Resources & Applications Facility (BRAF) at C-DAC, is an effort providing high-end supercomputing facility to the researchers working in the areas of Bioinformatics. The earlier supercomputing systems viz., PARAM Bio-Chrome, PARAM Bio-Blaze continue to cater to Indian scientific community. This year, PARAM Bio-Embryo has been added to BRAF that aims to aid in accelerated drug development and its allied research in a major manner.

It is evident that, the usage of HPC facilities has changed the gears from traditional Applications like Weather Forecasting to the latest demands of new Application areas like AI, Agriculture, Nano Science, and Quantum. C-DAC's NPSF, BRAF, and NSM Supercomputing Facilities have set an outstanding example of how the pandemic challenges such as COVID19 can't stop scientists and researchers from excelling in their work.

I assure that HPC-AI user community will continue to experience Next-Generation Supercomputers from C-DAC, offering state-of-art HPC-AI facilities for solving some of the challenging problems in the key areas of Science and Technology.

At last, I congratulate NPSF, NSM and BRAF teams of C-DAC, Pune for their achievements and relentless efforts in running the facility and their contribution to the mission.

Dr. Hemant Darbari
Director General, C-DAC

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

Message from Executive Director

Computational tools offer society a new problem-solving paradigm. Exascale computing further provide the capability to tackle challenges in scientific discovery and national security at levels of complexity and performance that previously were out of reach. They have the potential to provide accurate predictions of complex phenomena for realistic conditions. These computational tools offer the potential to rapidly produce optimized designs for systems, explore the limits of those designs, accelerate scientific discoveries, predict the behaviour of natural systems like the weather, analyze and plan complex operations involving thousands to millions of individual entities, and analyze & organize enormous amounts of data.

This year PARAM Yuva II completed 8 years of serving the supercomputing community of the nation. Since its commissioning, the National PARAM Supercomputing Facility (NPSF) has catered to more than 1200 users from around 132 scientific institutions. I thank all users of NPSF for their incessant support and their excellent contribution towards the Academic and Scientific community. The enriching experience earned throughout the journey has equipped C-DAC facing various computational challenges.

Continuing our journey of deployment of various HPC systems across the nation, as part of the national initiative under the National Supercomputing Mission (NSM) we are happy that the facilities, PARAM Shivay (837TF), PARAM Brahma (797TF), PARAM Shakti (1.66PF), PARAM Yukti (650TF) and PARAM Sangnak (1.3PF) are already functional at IIT Varanasi, IISER, Pune, JNCSAR and IIT Kanpur respectively. These are catering to the scientific community in an extensive manner making fast, and high-quality compute and tools available to researchers and scientists. The PARAM Bio Embryo (100TF) which is deployed at C-DAC, Pune is being used for extensive research on chemical as well as ayurvedic molecule formulations against COVID 19 from the word go.

A large number of applications ranging from flood prediction to seismic-based oil exploration to urban air and flood modelling, CFD based simulations are already being tested on the NSM resources deployed.
Collaboration with premier Scientific & engineering organizations will certainly help HPC team @ C-DAC in overcoming the challenges related to the development of next-generation Exascale systems development.

I wish you all the success for your future endeavors!

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

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1. About NPSF

Clusters at NPSF:

PARAM Siddhi-AI: Going to be operational from this Year, Peak Perf. 210 PF (AI) and 6.5 PF (Peak DP), Ranked 62nd in November 2020 in the 'Top500 Supercomputer List' published in November 2020' during Supercomputing Conference 2020 (SC 20) at United States.

PARAM Yuva II: Operational from the Year 2013, Peak Perf. 529.4 TFlop/s, Ranked 69th in June 2013 Top500

PARAM Yuva: Operational Year 2008-2012, Peak Perf. 54 TFlop/s, Ranked 69th in Nov. 2008, Top500

PARAM 10000: Operational Year 1998-2005, Peak Perf. 100 GFlop/s

1.1 Introduction

The National PARAM Supercomputing Facility (NPSF) is a result of more than two and half decades of effort in Research and Development (R&D) in High-Performance Computing (HPC) since C-DAC's inception. The National PARAM Supercomputing Facility was set up 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 to 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 Siddhi-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) and by far the fastest supercomputer developed in India, with a peak performance of 210 PFlops (AI), Rpeak of 6.5 PFlops (DP), and 4.6 PFlops Rmax (Sustained). Artificial intelligence aids research in advanced materials, computational chemistry & astrophysics, health care system, flood forecasting, and applications related to COVID-19 through faster simulations, medical imaging, and genome sequencing. In November 2020, PARAM Siddhi-AI ranked 62nd among the most powerful supercomputers in the world. It is built on the NVIDIA DGX SuperPOD reference architecture networking.

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 is among the latest addition to the series of prestigious PARAM series of supercomputers built in India. PARAM Yuva II is 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 ranked 69th in the Top500 list 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 the National Knowledge Network for accessing computing resources at NPSF. The scientific community uses 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 System Insights

Two Subclusters of PARAM Yuva II	
Subcluster-1	PARAM Yuva II: 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

Cluster of PARAM Siddhi-AI

PARAM Siddhi-AI:

Peak Perf. 210 Petaflop (AI)

Rpeak of 6.5 PFlops and 4.6 PFlop Rmax (Sustained)

42 nos. of NVIDIA DGX-A100 nodes

8x NVIDIA A100 Tensor Core GPUs each node

320 GB GPU memory

Infiniband HDR200 Interconnect Director switch

10.5 PiB storage with 250 GB/s throughput

500 TiB Flash-based storage and 10 PiB Disk-based storage.

Inferencing nodes with NVIDIA Tesla T4 GPUs.

1.3 Highlights

- Like every year, NPSF team participated to showcase NPSF during National Science Day celebration at C-DAC, Pune, on February 28, 2020. PARAM Yuva II model display attracted the most attention by school students and general public alike. In total, around 1800 visitors (Students from various colleges/institutions and schools) from Pune and nearby districts of Mumbai enjoyed the interactive technical sessions and visit to NPSF.

- NPSF sysadmins kept the system up and running and continued to provide quality services to the user community since COVID-19 pandemic started and lockdowns were imposed in March-2020.

- NPSF system and services have been utilized for SAMHAR COVID-19 Hackathon in May 2020. The setup included tools installation, environment setup, account creation and provisioning of access to the nodes through VPN and support.

- NPSF system has been planned to be utilized for Drug Discovery Hackathon 2020. The dedicated Sub cluster with required environment has been setup for the use by Drug Discovery Hackathon participants in July and August 2020

- NPSF system and services have been used for GPU Application Hackathon (GAH 2020) during September 2020.

- 42 nos. of NVIDIA DGX A100 systems (PARAM Siddhi-AI system compute) were installed at National PARAM Supercomputing Facility (NPSF) premise. The decision was so taken owing to non-readiness of DC at C-DAC Innovation Park and timelines for its completion were beyond last date for HPL result submission to November Top500 list. This was happened in September 2020.

- Accommodating 42 nodes posed a challenge in-terms of rack space availability and to mitigate aforementioned, existing PARAM Yuva I and Yuva II nodes (minimum quanta retained for functioning of NPSF services, including service and storage) were dismantled in September 2020

- NPSF HPC services was shut down for upgrading the power per rack capacity for placement of PARAM Siddhi-AI System compute nodes. The maintenance has been carried out from 1000Hrs 27th Sep, 2020 to 1230 hrs 30th Sep, 2020

- Server racks were identified to proportionately load cooling infrastructure including current operational load of systems at NPSF. Leftover rack units after consumption of 6*2 RUs were filled with custom made blanking panels. In addition to above for containment leading to efficient heat removal, very high RPM fans were procured in anticipation for heat removal from hot aisles and air circulation. This happened in October 2020.

- System was benchmarked with both single rail and dual rail IB connectivity to nodes as an assessment exercise for performance gained with various combinations of block sizes and process grid (P & Q).

- TOP500 Supercomputer List – November 2020 was announced on November 17, 2020 during SC20 placing “PARAM Siddhi – AI” at Rank 62, which is the highest ever ranking achieved by a PARAM supercomputer in the series.

- Out of 42 nodes, 2 mini-pods (Scalable units / SUs) constituting 5 nodes each were commissioned with all 8 IB(HDR 200) rails connected for compute fabric using single 40 port HDR 200 switch for each mini-pod respectively, to drive application benchmarking exercise with a semblance of architecture/ configuration dictated by NVIDIA for extracting performance. This was done in December 2020.

- 1PB SSD & NL-SAS based storage has been made available on two mini-pods of PARAM SIDDHI-AI system. This was done in December 2020.

- 2 nos. of NVIDIA DGX-1 systems which were installed in NPSF for PoC have been utilized for executing HPC / AI workloads by the users and were also used for PoC by the startup solutions for Safe City Project and for test setup of the NAADI project. NPSF sysadmins have supported the system from the system front.

- 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 2020, total 1698 invoices have been raised against consumed CPU Time of 43047643 CPU Hours. The e-money equivalent of the consumed CPU Time is 129142.98 debit units.

- Apart from NPSF operations, team members are faculty of Advanced Computing Training School (ACTS), C-DAC for PG Diploma course titled HPC System Administration (HPCSA). The diploma course is of 6 month duration with two batches in a year. As a faculty, delivering lectures, oversee and guiding during lab practice, conduction of end module lab exams are some of the obligations met.

- NPSF HPC services were interrupted due to failure in authentication service on 13th Mar, 2020. The downtime lasted for 11:30 Hours.

- NPSF HPC services were interrupted due to failure in the internet connectivity on 15th June, 2020. The downtime lasted for 7 hours.

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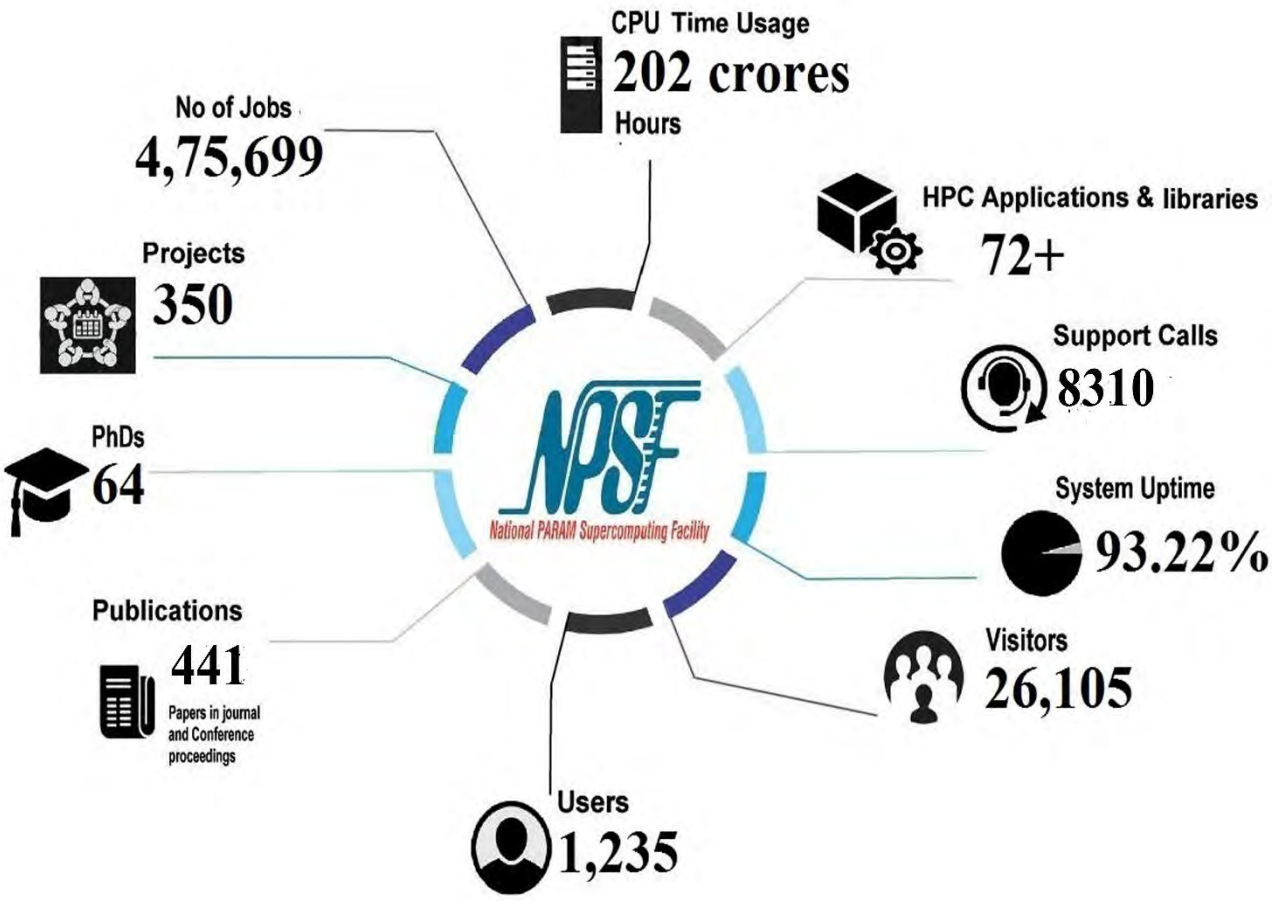
2. NPSF in Last 8 Years

Below are some of the NPSF statistics of last eight years i.e. Year 2013-20.

The statistics includes variation in cluster utilization, year-wise total number of projects, number of PhDs & publications produced using NPSF.



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2.1 NPSF in 8 years

C-DACs National PARAM Supercomputing Facility (NPSF) was established in March 1998 with the mandate to offer state-of-the-art High Performance Computing systems to various institutions and industries that need such a facility to process their diverse applications and resources, also to help them with the know-how and usage of such systems and proliferate HPC awareness in the country.

Major Events

- As part of the Provisioning of hybrid technologies in the National PARAM Supercomputing Facility and C-DACs Terascale Supercomputing Facility - A step towards Next-Generation HPC project, PARAM Yuva II system was launched in February 2013. The system performs at a peak of 524 TFLOPS, about 10 times faster than its predecessor i.e., PARAM Yuva. PARAM Yuva II relies on Intel Xeon Phi for its computing power, thus making it energy efficient than its predecessor, thus boosting the Flops per Watt index.

- The increase in peak compute power from 54 TeraFLOPS to more than half a PetaFLOPS is achieved without any increase in the electrical power and cooling required for the facility.

- Also, with this launch, C-DAC became the first R&D institution in India to cross the 500 TF milestone.

- Meticulous planning and coordination, consistent efforts, and use of expertise gained over the years helped in commissioning the in record time of 21 days, and the system was then offered as a resource to the HPC community.

- Benchmarking exercise for Top500 ranking was done for PARAM Yuva II system and achieved sustained performance of 386.7 TeraFLOPS and was ranked 69th in the June 2013 Top500 list.

- Energy consumed by supercomputers is measured at various Levels - L1, L2, and L3 - for purpose of reporting as part of the Green500 list. As the level increases, the accuracy and rigor of measurement exercise also increases. It is noteworthy that NPSF team has carried out Level 3 benchmark, and C-DAC became the second organization worldwide to have carried out the Level 3 measurement of Power versus Performance for the Green500 List.C-DAC achieved a significant milestone with PARAM Yuva II being ranked 1st in India, 9th in the Asia Pacific Region and 44th in the world among the most power-efficient computer systems with performance of 1,760.20 Mega Flops (MFs) per Watt as per the Green500 list released in November 2013

- To strengthen the security and accessibility of the PARAM Yuva II system, the system software architecture was re-architected, and the entire system was reinstalled with a near diskless, read-only setup.

- The security has been enhanced at various levels like data security, cluster level security, system level security, login access control and perimeter level security

- Revamping of cluster partitions was done in order to ensure optimal resource utilization and cater to the specific need of resources by group of users

- As an effort to apprise Chief Investigators (CI) of projects in NPSF, and also to serve as usage charges levied (not commercial), NPSF has started raising invoices for monthly CPU time utilization.

- Space Application Centre, ISRO has used NPSF PARAM Yuva II system extensively for their daily operational jobs run for consecutive 3 years with 99.4% of the day's successful job runs. The jobs have been managed to run in the maintenance period as well. NPSF team received acknowledgment from ISRO for the availability and maintenance of the resources and support provided.

- 2018 was a proud year for us, as the system uptime was maintained to 99.95%, which is the highest of all the years of NPSF. The efforts made by the team to keep the facility up and running all the time had shown the results.

- NPSF system and services have been utilized for SAMHAR COVID-19 Hackathon and GPU Application Hackathon and were planned to be used for Drug Discovery Hackathon in 2020. The setup included tools installation, environment setup, account creation and provisioning of access to the nodes through VPN and support.

- 42 nos. of NVIDIA DGX A100 systems were installed at National PARAM Supercomputing Facility (NPSF) premise. The decision was so taken owing to the non-readiness of DC at C-DAC Innovation Park, and timelines for its completion were beyond the last date for HPL result submission to November Top500 list. This was happened in September / October 2020.

- System was benchmarked with both single-rail and dual-rail IB connectivity to nodes as an assessment exercise for performance gained with various combinations of block sizes and process grid (P & Q)

- TOP500 Supercomputer List – November 2020 was announced on November 17, 2020, during SC20 placing "PARAM Siddhi–AI" at Rank 62, which is the highest ever ranking achieved by a PARAM supercomputer in the series.

System Management and Monitoring

- To test various policies and configurations before deploying on the actual PARAM Yuva II system, a similar setup has been created so that any evaluation of installation, configuration change or policy implementation can be tested before being placed into production

- Remote management was enabled for all the nodes in-order to manage them remotely even when OS is not booted or node crashed, also to perform power ON/OFF/Recycle remotely

- The PARAM Yuva II ecosystem is being monitored closely with the help of monitoring tools. Alerts are also in place to catch the attention on priority NPSF Web Portal: Feature-rich and user friendly

- NPSF web portal has been in place. It also serves as a collaborative environment for NPSF user community.

- On the development front, development/customization and installation of required tools for efficient use of the system and ease of monitoring and management of the facility have been done. This majorly included power-aware scheduling, customized monitoring tools, customized resource manager and scheduler, performance data collection framework, and many other tools and services. Automation of the many day-to-day tasks is also done.

System Utilization and Usage Policies

- Since the facility is shared by more than 1200 users across India, adequate mechanisms are put in place to ensure maximum throughput and optimal resource usage of the systems. The policies are made based on the system's capabilities, targeted use, and user demand for the resource. The policies are periodically monitored and changed if necessary.

- Dedicated Slot Booking Facility: Online Dedicated Slot Booking Facility was in place to address the need for dedicated resources by users. The dedicated slots have been provided to the users at regular intervals. Several users are greatly benefitted by the use of DSBF.

- For the processing of a large number of cores (512 to 1024) jobs with less wall time, a new execution queue BURSTq was introduced on 9th Sept. 2016. The jobs requiring more than 512 and less than 1024 cores for a maximum of 17:55:00 Hrs wall time jobs were made to route to this queue. Introduction of this queue helped a lot for processing of BIG jobs.

- The usage reports are generated on a monthly basis and help us to understand the usage patterns, which help us in fine-tuning the usage policies.

- NPSF sysadmins kept the system up and running and continued to provide quality services to the user community since COVID-19 pandemic started and lockdowns were imposed in March-2020.

User Support

- Keeping in view the practice followed worldwide, a scheme called the Technical Affiliation Scheme(TAS) is in place with the objective of encouraging the potential users of high-performance computing resources in a cost-effective way and also provides a technically congenial environment to the researchers using NPSF. NPSF team has been supporting a large pool of HPC users belonging to various application domains and profiles via e-mail, chat, telephonic support, sharing the user terminal, and in person.

Workshops, Lectures, and Talks

- From the last 4 years, NPSF team members are engaging themselves in delivering lectures, oversee and guide during lab practice sessions, and conducting end module exams, for PG Diploma on HPC System Administration (HPC-SA), under Advanced Computing Training School (ACTS), C-DAC. This is six monthly, twice in a year activity.

- In the last 8 years, NPSF team members have organized 9 workshops and delivered more than 20 talks in different forums.

- NPSF Team, in collaboration with NVIDIA, has arranged 5 days long online training on PARAM Siddhi-AI system. More than 200 participants have attended the training.

Breakdowns

- PARAM Yuva II cluster is being managed without any AMC from last 4 years. NPSF team has been maintaining the cluster on best effort basis. There have been breakdowns in the facility due

to failures in IT and non-IT infrastructure. In the recent past, NPSF PARAM Yuva II services were largely affected due to failures in the IT infrastructure, mainly due to storage failure. In addition to the failures in the IT-Infrastructure, there have been unplanned service breakdowns due to non-IT infrastructure failures as well, mainly due to power sub-system failure. The total downtime in the last 8 years is 7% out of which 50 % of the downtime has been added in this year which is the downtime accounted due to storage subsystem failure. The total downtime in the last 8 years is 6.8% out of which 40% of the downtime has been added in the last year which is the downtime accounted due to storage subsystem failure.

Acknowledgment

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

- Also, we express our sincere gratitude to the members of the PRSG committees who have guided and supported the activities of NPSF.

- Our sincere thanks to our Director General, Executive Director, and Head of the Department, who have made sure that NPSF continues to offer services in spite of funding issues.

- Finally, we acknowledge the support received from the ever-growing NPSF user community to make this journey successful.

2.2 8 Years Statistics

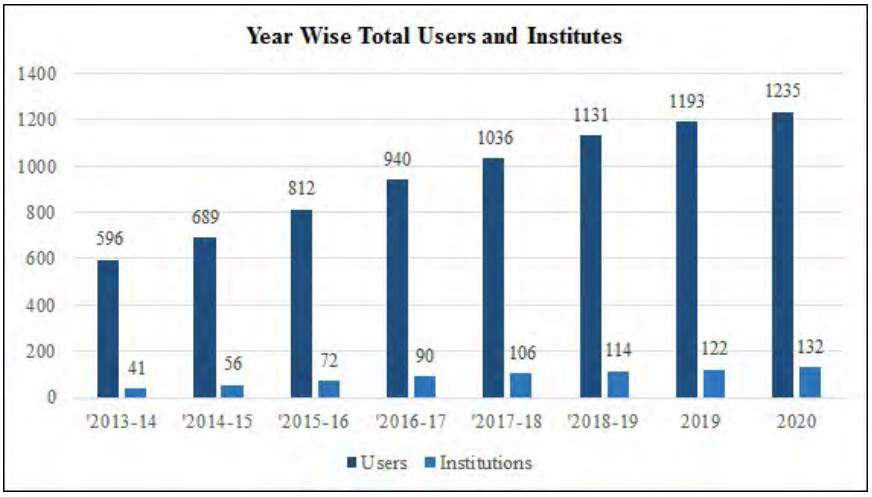


Table: Year- wise total users and institutions

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

The above bar graph shows growth in the count of NPSF users and institutes affiliated to NPSF. It is noteworthy that the number of users has more than doubled, and a number of institutions has tripled in the last 8 years.

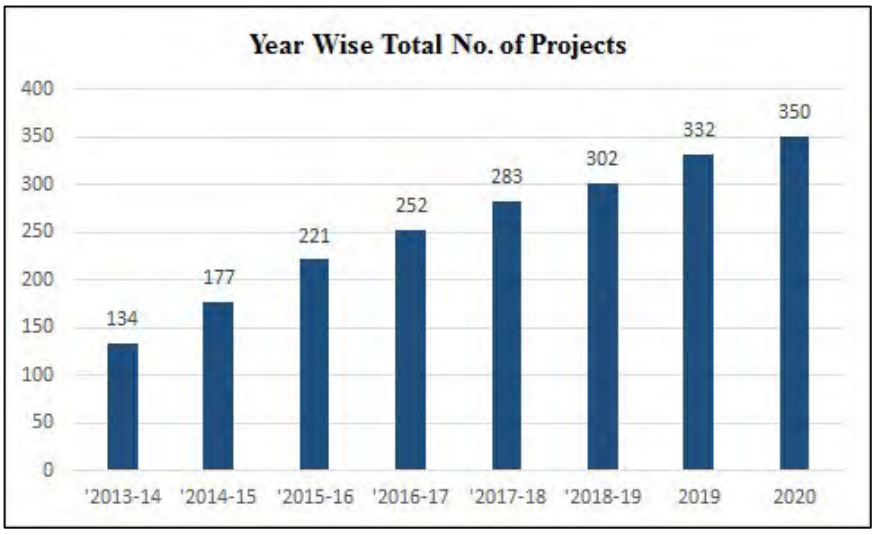


Table: Year- wise total number of projects

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

In the above bar graph, substantial growth in the number of projects registered with NPSF in the last 8 years.

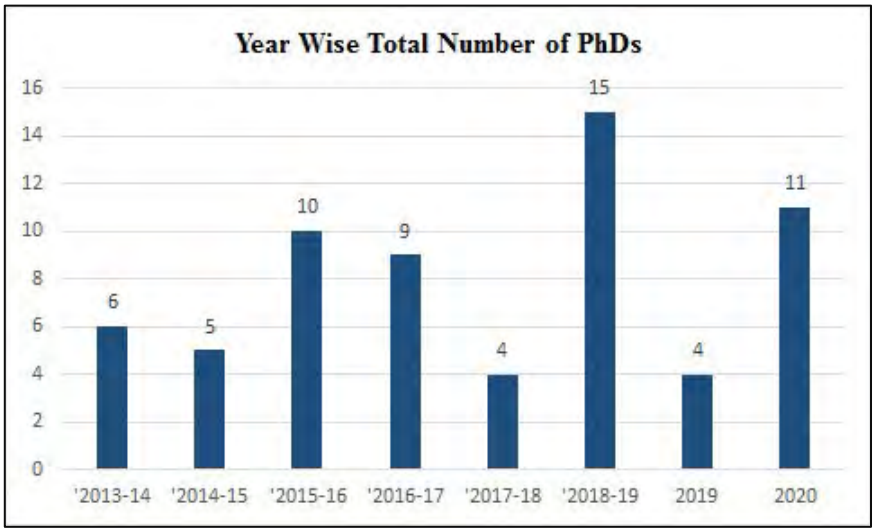


Table: Year wise number of PhDs

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

The above graph shows the number of PhDs completed using the NPSF PARAM Yuva II system. In the last 8 years, 64 PhDs have been completed using the NPSF PARAM Yuva II system. This also includes 11 PhDs awarded last year.

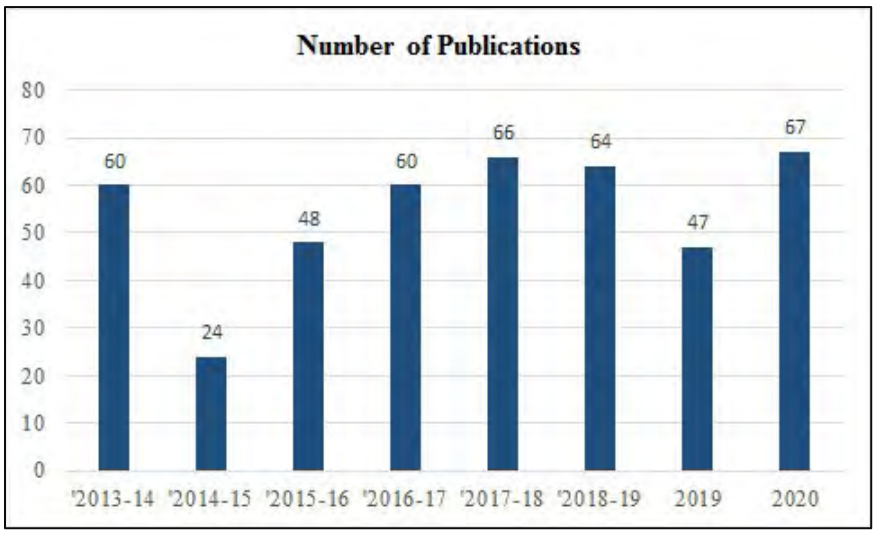


Table: Year- wise number of publications

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

NPSF users publish the publications in the journals where they duly acknowledge the NPSF PARAM Yuva II system. The total number of publications using the system is 442, and every year except 2014-15, nearly fifty or more publications are published in the reputed journals.

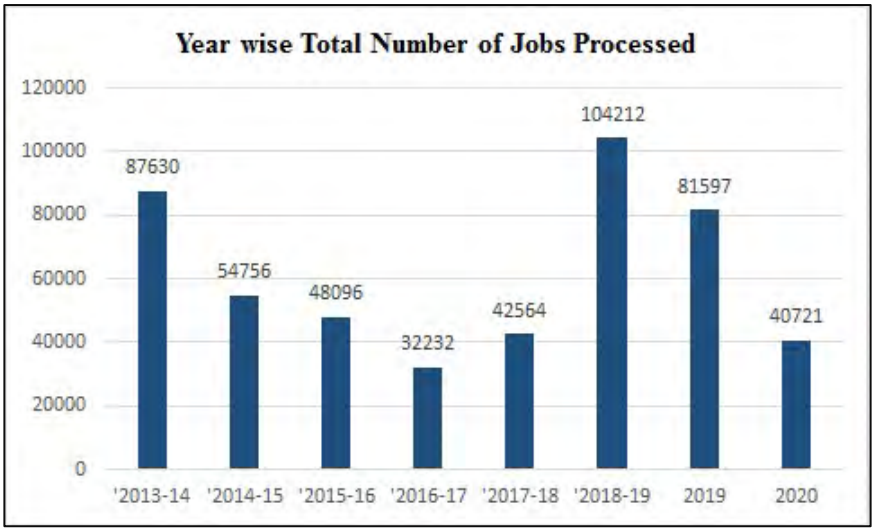


Table: Year-wise number of jobs processed

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

Thetotal number of jobs processed using NPSF PARAM Yuva II system is near to 4.75 Lac in the last 8 years.

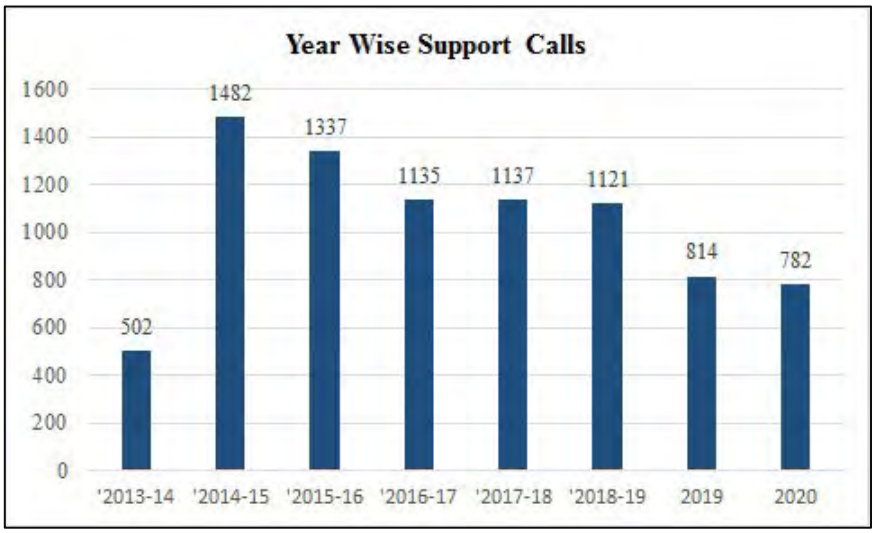


Table: Year-wise number of support calls

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

The above graph shows the year-wise number of support calls raised by NPSF users over e-mail for the help they require while on-boarding / using the system. The calls are duly resolved, and users are notified over e-mail about the resolution. More than 8310 calls have been attended so far.

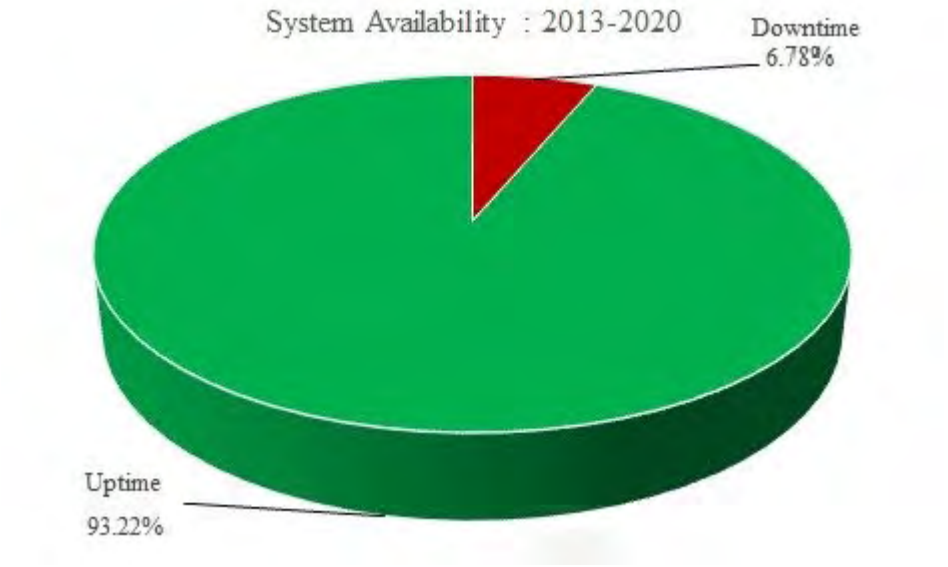
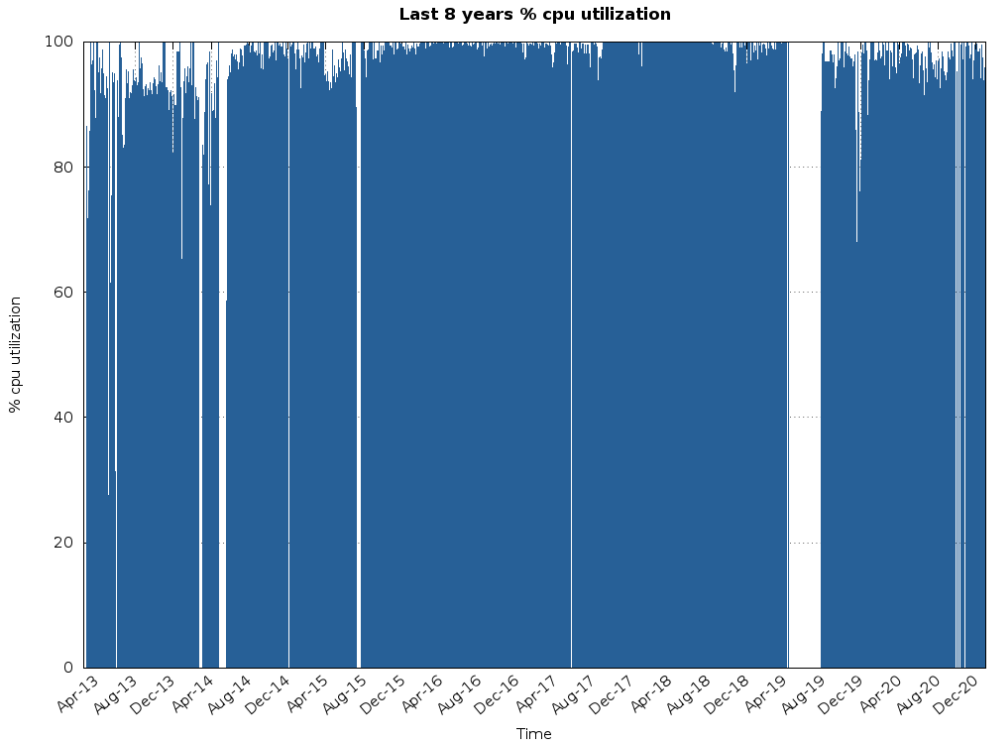


Table: System availability

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

The pie chart is an indicator of system uptime (availability) which is one of the most important aspects of the HPC facility. NPSF PARAM Yuva II system has 98.92% of the uptime over last 8 years.



% CPU utilization is calculated as % of CPU cores used out of available CPU core. This utilization is recorded every minute in the database. The above GNU Plot shows the utilization of 90% and above most of the time over the period of 8 years. This graph is also indicative of the very high utilization of the system consistently. The gaps in the plot indicate the system's maintenance period and, a few times, the non-availability of the stats.

3. PARAM Siddhi-AI System

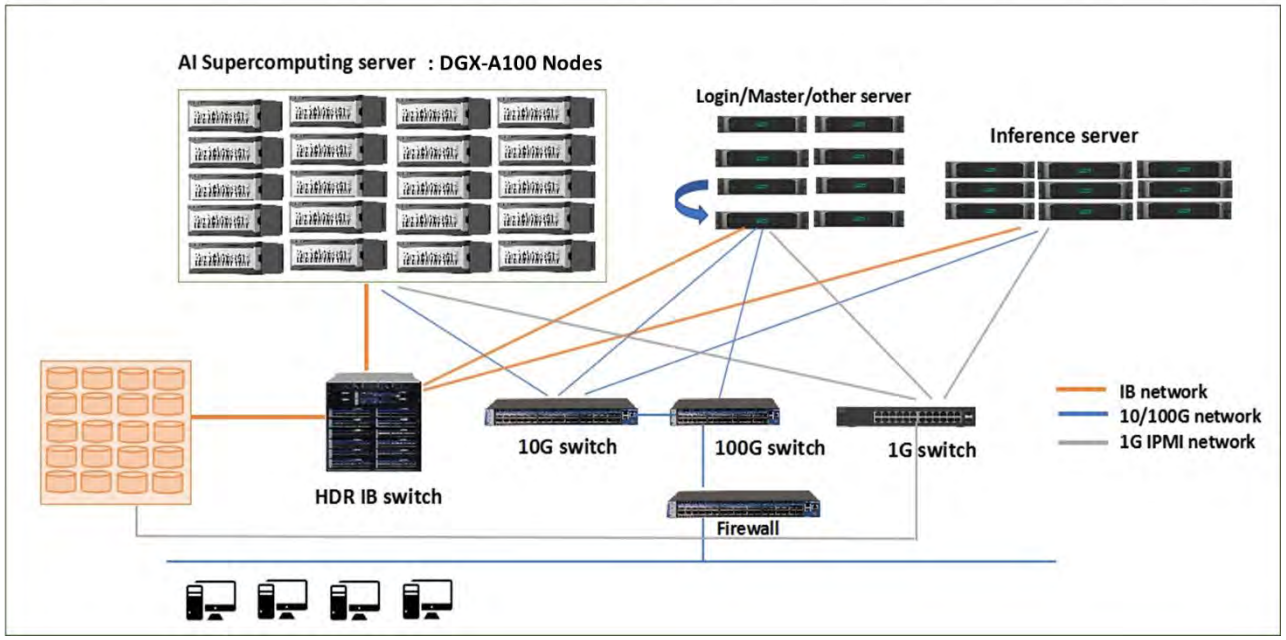
3.1 Introduction

NATIONAL SUPERCOMPUTING MISSION
INFRASTRUCTURE | APPLICATIONS | R&D | HRD

PARAM Siddhi-AI is a high-performance computing-artificial intelligence (HPC-AI) and by far the fastest supercomputer developed in India with peak perf. of 210 Petaflop (AI), Rpeak of 6.5 PFlops, and 4.6 PFlops Rmax (Sustained). Artificial intelligence aids research in advanced materials, computational chemistry & astrophysics, health care system, flood forecasting, and applications related to COVID-19 through faster simulations, medical imaging, and genome sequencing. In November 2020, PARAM Siddhi-AI ranked 62nd among the most powerful supercomputers in the world. The system is built on the NVIDIA DGX SuperPOD reference architecture.

The system has 42 nos. of NVIDIA DGX-A100 nodes. Each node has 8x NVIDIA A100 Tensor Core GPUs, and the total GPU memory is 320 GB. The system is equipped with Infiniband HDR200 Interconnect Director switch. The storage is 10.5 PiB with 250 GB/S throughputs having 500 TiB Flash-based storage and 10 PiB Disk-based storage. The system is also having Inferencing nodes with NVIDIA Tesla T4 GPUs.

PARAM Siddhi-AI Schematic Diagram:



3.2 Activities

Installation and Commissioning at NPSF :

- 42 nos. of NVIDIA DGX A100 systems were installed at National PARAM Supercomputing Facility (NPSF) premise. The decision was so taken owing to non-readiness of DC at C-DAC Innovation Park, and timelines for its completion were beyond the last date for HPL result submission to November Top500 list.

- Accommodating 42 nodes posed a challenge in terms of rack space availability, and to mitigate the aforementioned, existing PARAM Yuva I and Yuva II nodes (minimum quanta retained for the functioning of NPSF services, including service and storage) were dismantled

- Due to the dense compute per node, mounting and rack placement was primarily dictated by power rating and even distribution across UPS sources and cooling infrastructure. In consultation with electrical personnel, the scheme was arrived to populate 2 DGX per rack, totaling 13KW against a rated 14KW per rack. For better inlet CFM, DGX systems were mounted, leaving 6 RUs from the bottom.

- Server racks were identified to proportionately load cooling infrastructure, including current operational load of systems at NPSF. Leftover rack units after consumption of 6*2 RUs were filled with custom-made blanking panels. In addition to the above for containment leading to efficient heat removal, very high RPM fans were procured in anticipation of heat removal from hot aisles and air circulation.

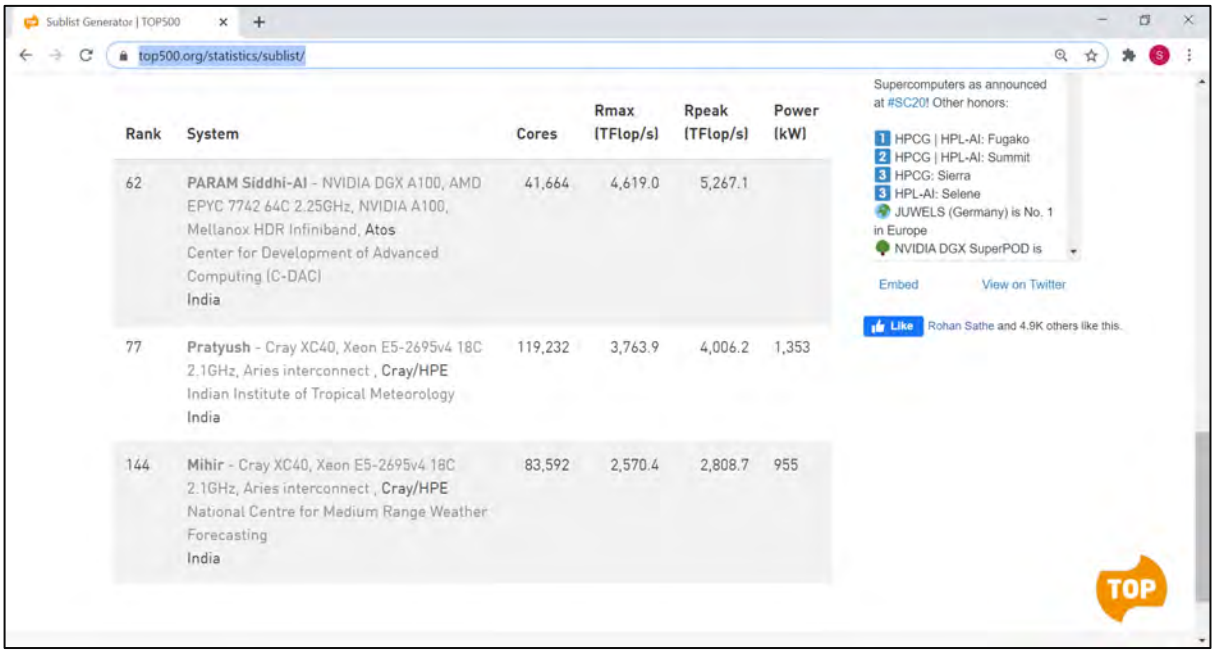
HPL Benchmarking:

The system was benchmarked by running the HPL benchmark.

```
================================================================================
T/V                N    NB     P     Q               Time                 Gflops
--------------------------------------------------------------------------------
WR03L2R2     1317888   288    21    16             330.37          4.619e+06
--------------------------------------------------------------------------------
||Ax-b||_oo/(eps*(||A||_oo*||x||_oo+||b||_oo)*N)=        0.0000013 ..... PASSED
================================================================================

Finished      1 tests with the following results:
              1 tests completed and passed residual checks,
              0 tests completed and failed residual checks,
              0 tests skipped because of illegal input values.
--------------------------------------------------------------------------------

End of Tests.
================================================================================
```



- TOP500 Supercomputer List – November 2020 was announced on November 17, 2020, during SC20 placing “PARAM Siddhi – AI” at Rank 62, which is the highest ever ranking achieved by a PARAM supercomputer in the series.

- In a parallel track, placing “PARAM Siddhi-AI” is today the largest and fastest Supercomputer in India. The system has been ranked as the no. 1 system in the TopSc.in list (list of the most powerful supercomputers in India)

Storage commissioning:

- Out of 42 nodes, 2 mini-pods (Scalable units / SUs) constituting 5 nodes each were commissioned with all 8 IB(HDR 200) rails connected for compute fabric using a single 40 port HDR 200 switch for each mini-pod respectively, to drive application benchmarking exercise with a semblance of architecture/ configuration dictated by NVIDIA for extracting performance.

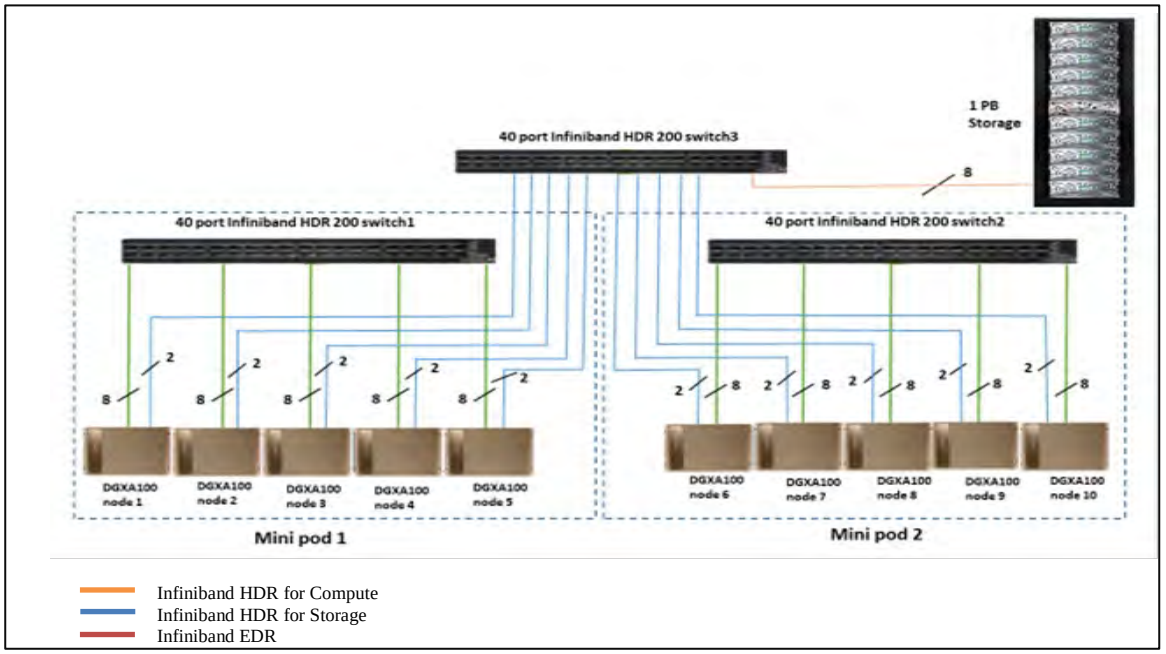
- 1PB SSD & NL-SAS-based storage has been made available on two mini-pods of PARAM SIDDHI-AI system. Highlights of which are :

    - DDN storage controllers connected to EDR switch using FDR cables

    - Reconfiguration of ethernet port to InfiniBand port (dedicated interface for storage) done on the DGX-A100 nodes in mini-pod

    - One IB HDR port from each DGX-A100 node (10 nos. of them) is connected to a separate (dedicated) IB HDR switch using HDR cables for storage delivery

    - EDR and HDR IB switch uplinked using 4 nos. of EDR cables (4 IB rails)



Application Benchmarking:

Assessment of compute prowess by way of application benchmarking from across various domains was undertaken.

List of applications being benchmarked are:

#	Application	Status
1	GROMA CS	Completed
2	LAMMPS	Completed
3	NAMD	Completed
4	AMBER	In Progress
5	Relion	In Progress
6	Quantum Espresso	In Progress
7	VASP	In queue
8	ICON	In queue
9	FUN3D	In queue
10	SPECFEM3D	Multi-node benchmarking runs ongoing
11	RTM	In queue
12	CHROMA	Single node setup completed
13	GTC	In queue
14	MILC	Completed
15	WRF	Completed
16	PyTorch-Object Detection - Light (SSD)	Completed
17	PyTorch-Object Detection - Heavy (MaskRCNN)	Completed
18	PyTorch-Translation - GNMT	Completed
19	PyTorch-Translation - Transformer	Completed
20	TensorFlow-MiniGo	Completed
21	TensorFlow-Image Classification	Completed

Application Research Fields (Domains) and Applications, Frameworks, Tools, and Libraries

List of Application Research Fields:

- Computational Materials Sciences
- Computational Fluid Dynamics
- CFD: Scalable Solvers for Compressible Navier-Stokes Equation
- Flow-induced Vibration (FIV)
- Computational fluid dynamics, bluff-body flow simulation
- Aerospace Engineering

- Supersonic Air Intake (Computational Fluid Dynamics)
- Flood prediction
- MultiGPU FFT
- Benchmarking and speed optimization of indigenous quantum simulator
- Text to Text machine translation using neural network and Machine Learning for Lok Sabha and SSMT project
- Automatic Speech Recognition (ASR)
- Medical Imaging (Specifically Ultrasound Imaging)
- Computer Vision and Image Processing
- Computer vision
- Speech Processing
- End2End Speech synthesis and Lip Syncing,
- Speech Synthesis / Machine learning
- End2End Speech synthesis and Prosody manipulation
- Speech Technology
- Text-to-speech synthesis in end-to-end framework

List of Applications, Frameworks, Tools, and Libraries

ANUGA Hydro	HTK	Finite Element Method based incompressible flow solver (codes)
CUDA Toolkit	FLAME Solver which uses MPI	Jarvis
cuDNN	Flask	Kaldi
Espnet	Gmsh	Keras (Tensorflow)
FFTK	Gstreamer	MPI libraries
NeMo	PyQT	Scikitlearn
OpenCV	Python	Sentencepiece
OpenFOAM	PyTorch	Subword
OpenNMT and DarkNet YOLO	Qiskit	TARANG
Paraview	Regent	Tecplot
Tensorflow	VTK	Waveglow

User and Institution Details:

- Total Number of Users: 71
- Internal Users (C-DAC): 25
- External Users (from other institutes): 46
- NVIDIA, ATOS (Benchmarking Team): 25
- Number of Institutes including C-DAC: 8

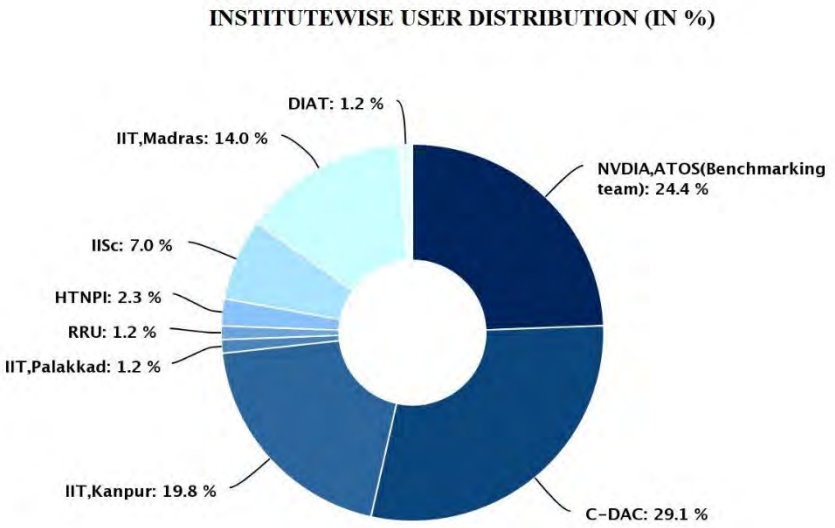


Table : Institute wise User Distribution

Institution	Users
NVIDIA, ATOS (Benchmarking team)	21
C-DAC	25
IIT, Kanpur	17
IIT, Palakkad	1
IIT, Madras	12
DIAT	1
RRU	1
HTNPI	2
IISc	6

Bootcamps in collaboration with NVIDIA:

i) OpenACC Bootcamp Phase 1: (56 participants and using 8 nodes)

56 participants have been on-boarded the system. Environment setup, Close monitoring, and continuous user support to all the participants have been provided.

ii) OpenACC Bootcamp Phase 2: (81 participants and using 2 nodes)

By enabling the MIG feature of the A100 GPUs, we have provided the GPU instances to the participants, and we could accommodate 81 participants on only 2 DGX-A100 nodes without any issues. This otherwise would have required 11 compute nodes. The setup included MIG enablement, GPU instance creation, compute instance creation, tools installation, environment setup, user creation, and provisioning of access to the nodes through

VPN. Preparation of System usage manual for the boot camp. 81 participants have been on-boarded on the system along with and support has been provided.

iii) AI F or Science Bootcamp: (84 participants and using 4 nodes)

By enabling MIG feature of the A100 GPUs, we have provided the GPU instances to the participants, and we could accommodate 84 participants on only 4 DGX-A100 nodes without any issues. The setup included MIG enablement, GPU instance creation, compute instance creation, tools installation, environment setup, user creation, and provisioning access to the nodes through VPN. Preparation of System usage manual for the bootcamp. 81 participants have been on-boarded the system, and support has been provided.

Training:

As part of series of training programs focused around PARAM Siddhi-AI system, online training in partnership with NVIDIA has been conducted from 15th March 2021 to 19th March 2021. 203 participations, including PARAM Siddhi-AI users from various research and academic institutes, have attended the training. In training, HPC-AI experts from NVIDIA have delivered talks ranging from CUDA computing, NVIDIA A100 GPU, and various AI tools to demo and hands-on applications on GPU.

3.3 Work Report Summary

1. "15 classes, including vehicles and other objects Detector for Indian roads" by Amit Raj, Joint Director, ramit@cdac.in , C-DAC

2. "Porting and Scaling of FFTK and TARANG to PARAM Siddhi-AI", Mahendra K. Verma, Professor, mkv@iitk.ac.in, IIT Kanpur

3. "Optical character recognition (OCR) for Indian Languages," Ronak Shah, Joint Director, ronaks@cdac.in, C-DAC

4. "Transitions in flow past a circular cylinder", Sanjay Mittal, Professor, smittal@iitk.ac.in, IIT Kanpur

5. "Learning with massive noisy face dataset for obtaining and training a clean dataset for Face Recognition", Kapil Mehrotra, Joint Director, kapilm@cdac.in, Karan Khajuria, Project Engineer & Vivek Chandra Project Engineer, C-DAC Pune

6. "Indexing Billion of face features (for similarity) on GPU", Kapil Mehrotra, Joint Director, kapilm@cdac.in, Karan Khajuria, Project Engineer & Vivek Chandra Project Engineer, C-DAC Pune

7. "Exploration of LINUX tools and HPC using CUDA", Dr. Manish Modani, Principal Solution Architect, ganinampelly979@gmail.com, NVIDIA

8. "Numerical Investigation of Flow inside a 3D Supersonic Y Duct", Dr. Sanjay Mittal, Professor, arkadipd@iitk.ac.in, IIT Kanpur

9. "FLAME Solver – Scalable Asynchrony-Tolerant Solver for Compressible Navier-Stokes Equations", Dr. Konduri Aditya, Assistant Professor, konduriadi@iisc.ac.in , IISc, Bangalore

10. "Automatic Speech Recognition", S. Umesh, Professor, umeshs@ee.iitm.ac.in, IIT Madras

11. "Scalable finite-element based real-space algorithms for quantum mechanical modeling of materials at extreme-scale", Dr. Phani Motamarri, Assistant Professor, phanim@iisc.ac.in, IISc, Bangalore

12. "Application performance and analysis at Scale. The applications include WRF, GROMACS, SPECFEM3d etc. These applications performances, first time, analyzed on multi-node, multi-GPUs on PARAM SIDDHI AI system", Dr. Manish Modani, Principal Solution Architect, mmodani@nvidia.com, NVIDIA

13. "Automated Lung Ultrasound Image Analysis", Dr. Mahesh Raveendranatha Panicker, Assistant Professor, mahesh@iitpkd.ac.in, IIT, Palakkad

14. “Design and development of End-to-End Automatic Speech Recognition system for Hindi & Indian English languages using cutting-edge deep learning algorithms, frameworks, and pipelines”, Mahesh Bhargava, mbhargava@cdac.in, C-DAC

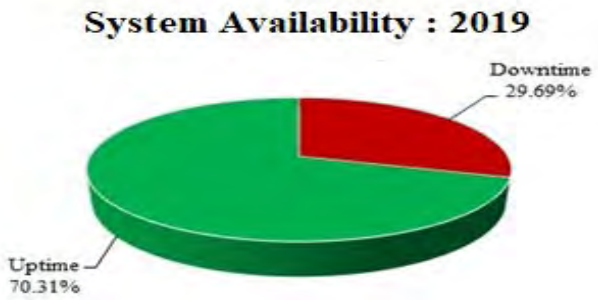
4. Statistics of PARAM Yuva II

In Year 2020: Users added: 42; Institutions added: 10; Jobs processed: 40721

4.1 System

System availability

The pie chart is an indicator of system uptime (availability) which is one of the most important aspects of HPC facility. It can be seen that the system availability has increased to 98.92% from 70.31%, as compared to last year one.



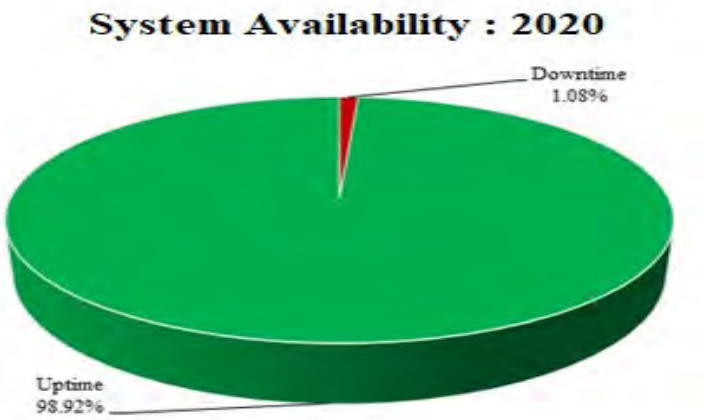
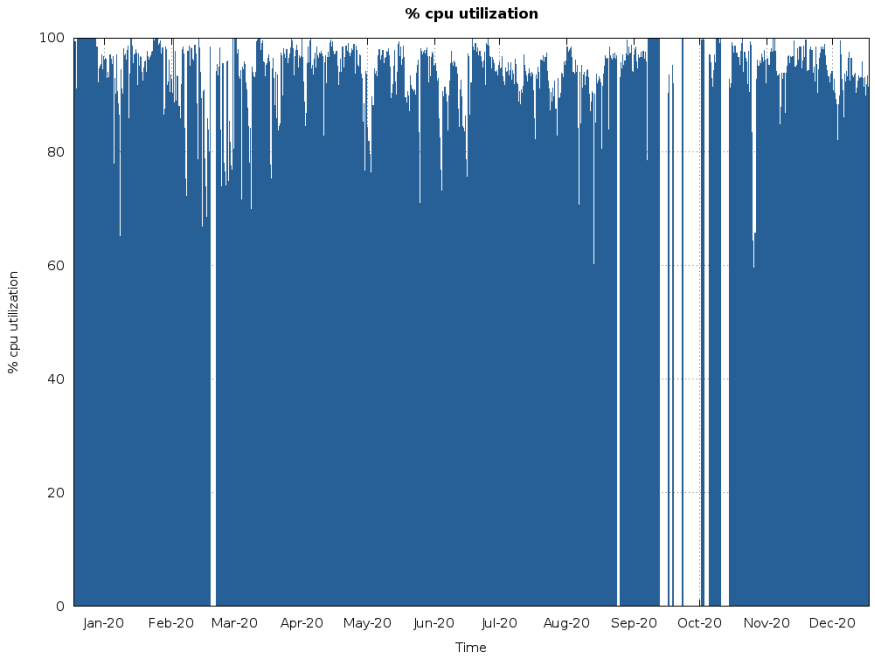


Table: System availability

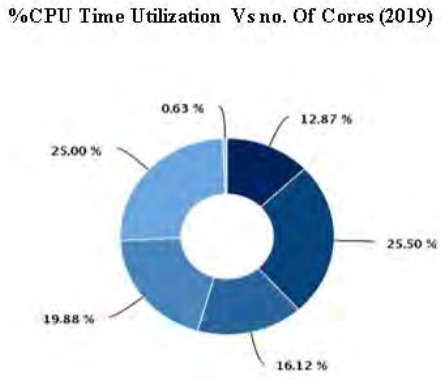
Duration	Total Time	Downtime
1 Jan'19 - 31 Dec'19	365 Days (total : 8760 Hours)	108.35 Days (2600 Hours, 34 Minutes)
1 Jan'20 – 31 Dec'20	366 Days (total : 8784 Hours)	3.92 Days (93 Hours)

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 above GNU plot, It can be seen that the system utilization most of the times remained above 90% throughout the year. The gaps in the plot are indicative of non-availability of the system and few times, non-availability of the data. The gap seen between 8th April to 22nd July, 2019 is the indicator of non-availability of the system due to failure of the storage system at NPSF.



CPU time utilization w.r.t. job sizes



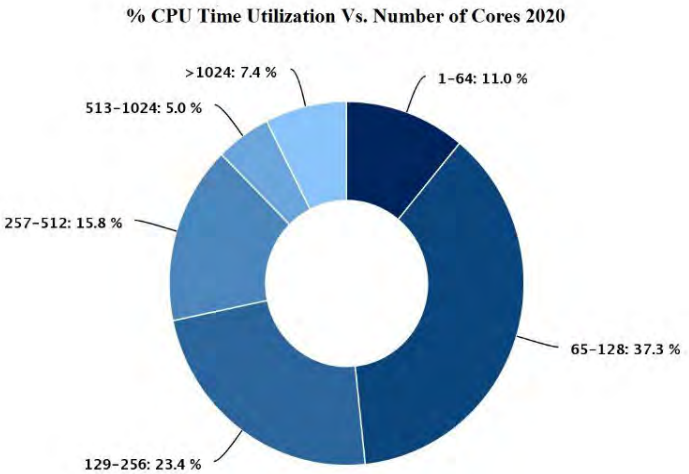


Table: CPU time utilization w.r.t. Job sizes

	CPU time utilized (in seconds)	
Job Sizes	**2019**	**2020**
1-64	17353205383	16013713917
65-128	34370568320	54380930324
129-256	21729859504	34080972440
257-512	26800724448	23042286320
513-1024	33704459698	7299652256
>1024	845818160	10836073472

Above doughnut indicates % distribution of CPU Time among different job sizes (binned by number of cores). It can be seen that there is 10% increase in use of CPU Time by big jobs (jobs requiring more than 64 cores).This is also indication of increase in % of capability computing.

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

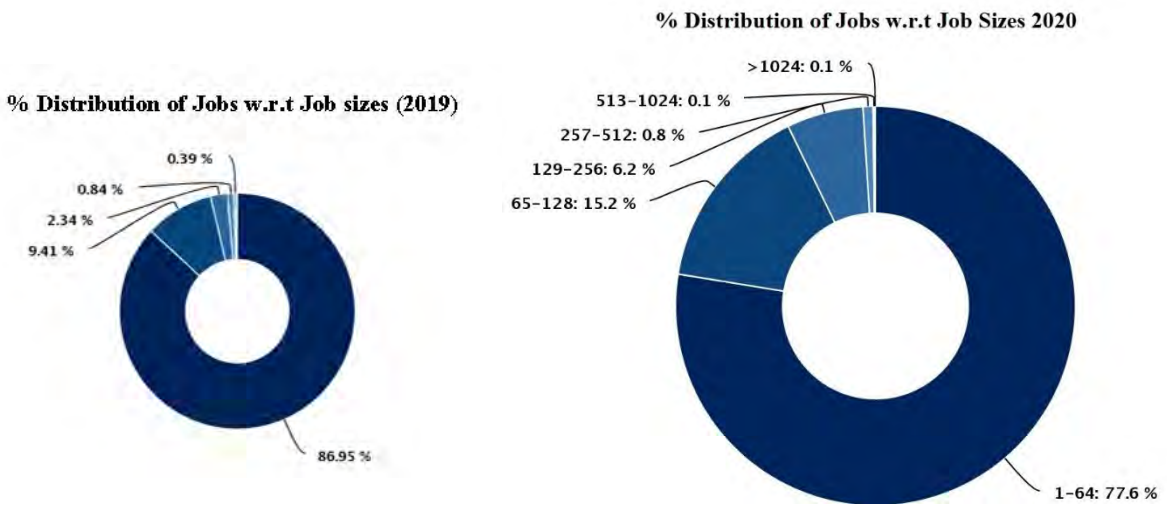


Table: Distribution of jobs w.r.t. Job sizes

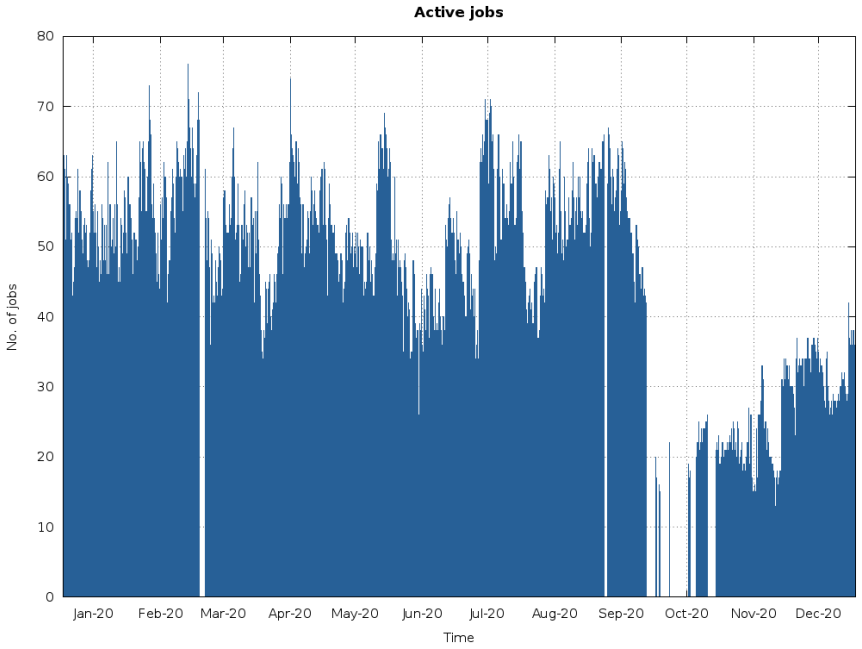
	Job Count	
Job Sizes	**2019**	**2020**
1-64	70566	31590
65-128	7634	6209
129-256	1901	2525
257-512	680	331
513-1024	318	50
>1024	62	23

Above doughnut indicates % distribution of number of batch jobs binned by the number of cores.

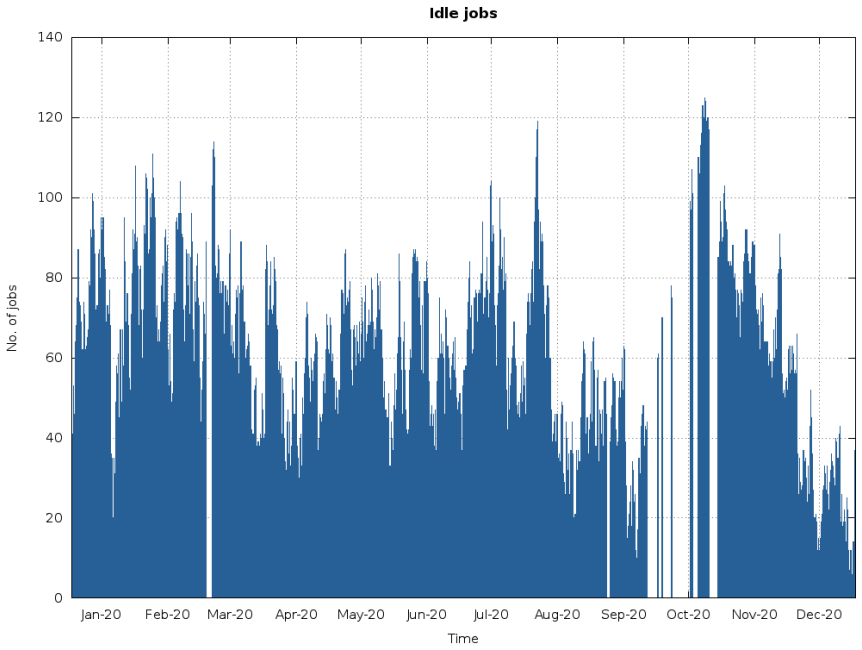
Active jobs, idle jobs & system backlog

A job on NPSF HPC system is a construct comprising of 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 presents figures for 1) Active jobs currently being processed, & 2) Idle jobs eligible for execution and waiting to be allocated the resources requested. The effect of the 105 day log maintenance is seen in both the GNU plots.

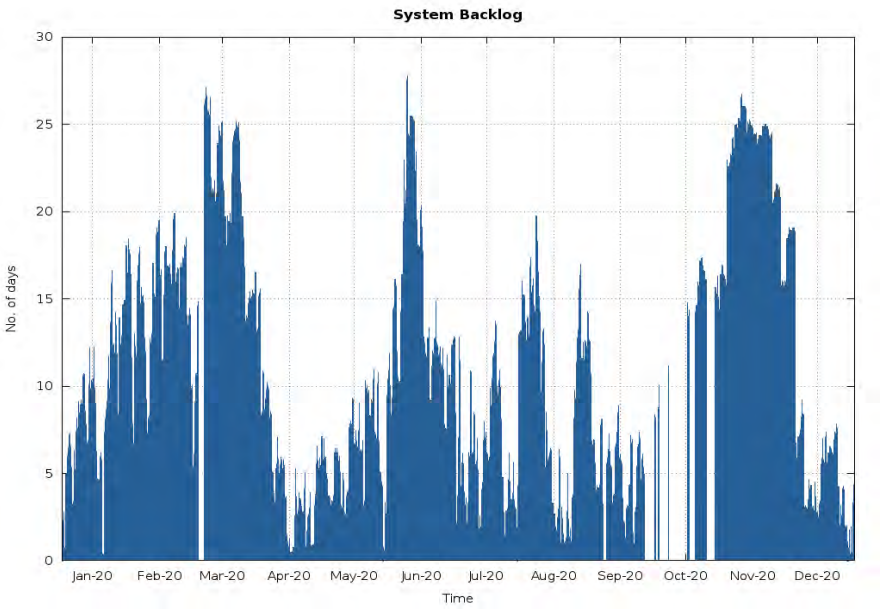
Active jobs



Idle jobs



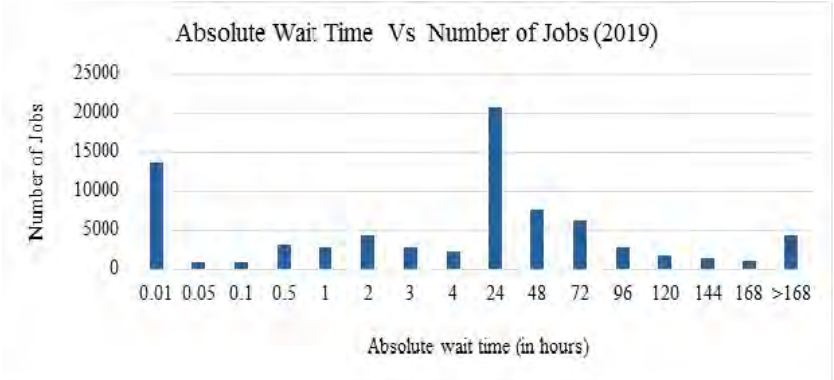
System backlog



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.

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.



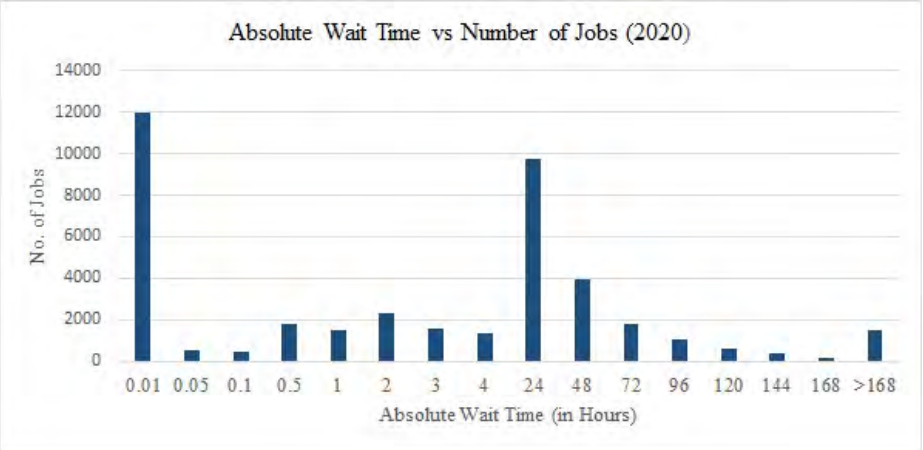
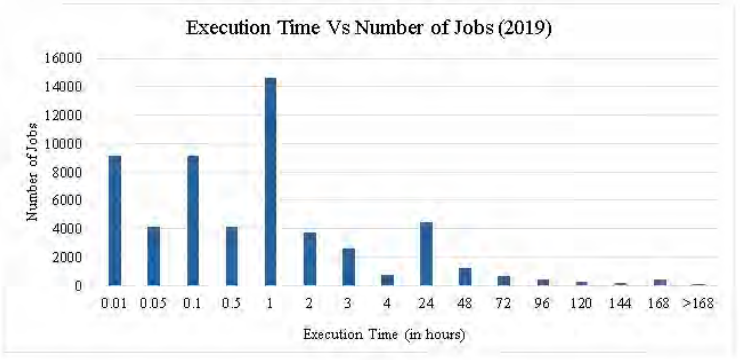


Table: Absolute wait time Vs no. of jobs

	No. of jobs	
Absolute wait time (in hours)	**Number of Jobs(2019)**	**Number of Jobs(2020)**
0.01	13704	11957
0.05	832	524
0.1	779	475
0.5	3171	1835
1	2837	1498
2	4274	2353
3	2739	1580
4	2455	1340
24	20578	9763
48	7574	3967
72	6152	1800
96	2687	1044
120	1854	603
144	1456	380
168	1073	206
>168	4273	1502

Above presentation is irrespective of job size.

Execution Time Vs Number of Jobs



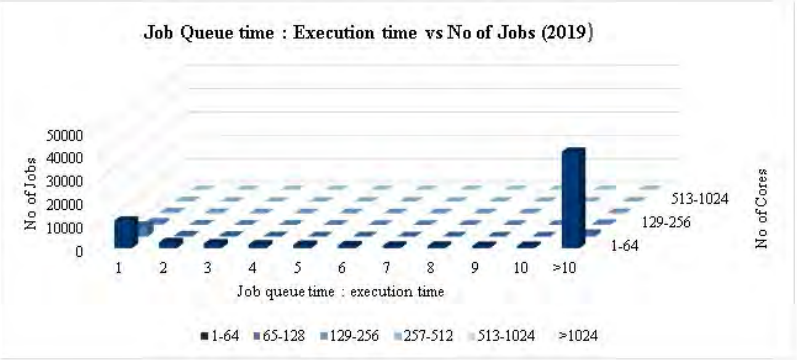
Above graph represents execution time of the jobs in hours

	Number of Jobs	
Execution Time (in hours)	**Number of Jobs (2019)**	**Number of Jobs (2020)**
0.01	9155	3841
0.05	4143	2749
0.1	9155	7538
0.5	4143	3865
1	14657	3776
2	3745	2977
3	2577	679
4	742	4630
24	4477	1179
48	1244	772
72	680	400
96	402	361
120	228	312
144	209	541
168	441	47
0.01	9155	3841

Relative measure of job wait time with respect to its 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.



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.

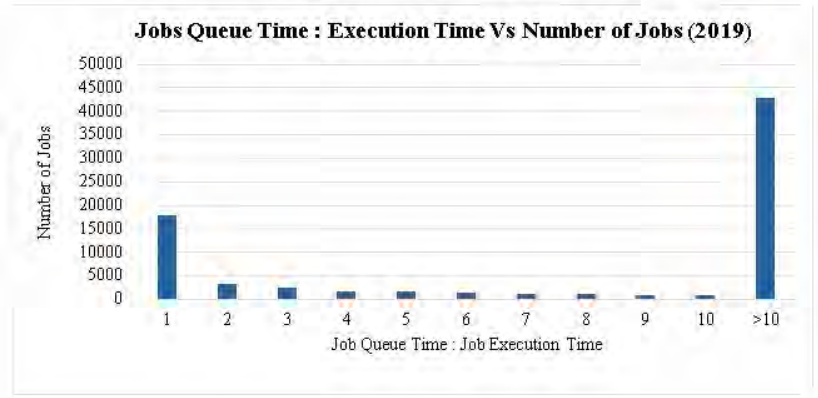
This segregation is made because job count for 1 to 64 CPU cores, being very high, diminishes bars for other job sizes, thus making observable distance between them nondescript.

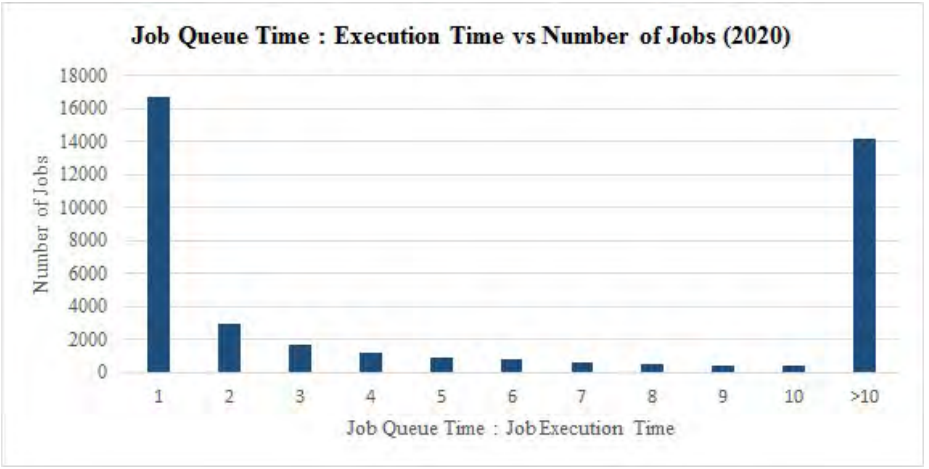
Table: Ratio of job waittime: execution time Vs number of jobs

2019	1	2	3	4	5	6	7	8	9	10	>10
1-64	11785	2525	1953	1541	1407	1166	1007	957	898	927	41257
65-128	4497	469	271	181	125	111	85	66	41	38	1073
129-256	968	145	88	44	42	28	22	22	17	10	388
257-512	377	106	31	10	11	11	6	5	4	2	81
513-1024	171	24	12	2	0	1	2	3	1	0	84
>1024	2	1	1	0	0	0	0	0	0	0	37

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

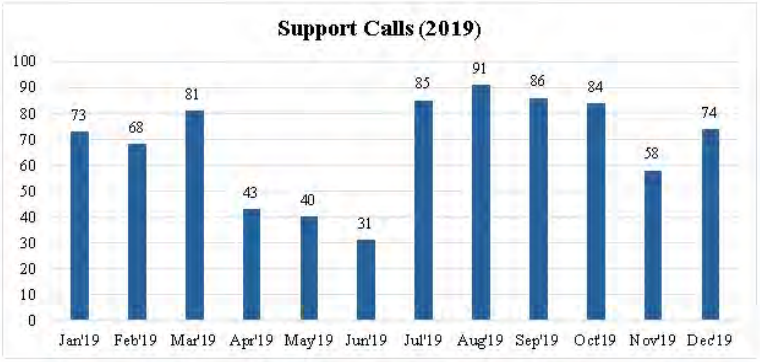




It can be seen from the graph that only 24% of the jobs have spent less than or equal amount of time in the queue as of its execution time (irrespective of job sizes). The percentage of turnaround time of the jobs has decreased by 8%, as compared to last year.

User support calls

Below Bar Graph shows the month wise distribution of support calls raised by users throughout the Year 2020.



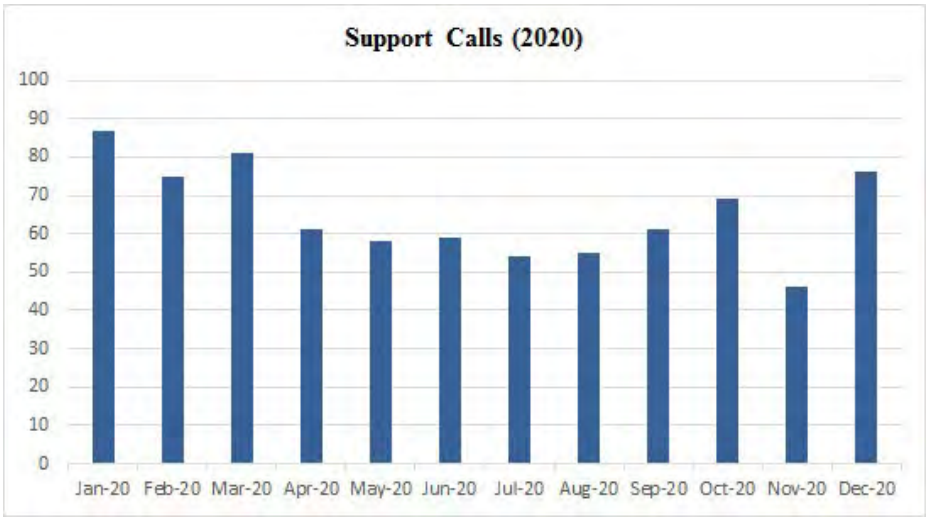


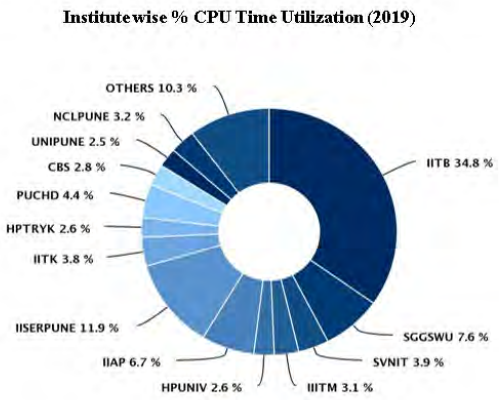
Table: Number of support calls

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
2019	73	68	81	43	40	31	85	91	86	84	58	74
2020	87	75	81	61	58	59	54	55	61	69	46	76

4.2 Users and Institutes

Institute wise CPU time utilization

User's Jobs running over the cluster consume 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 2019 and 2020 plots, Jobs submitted from users of IIT Bombay are continuously consuming the max. % of CPU Time.



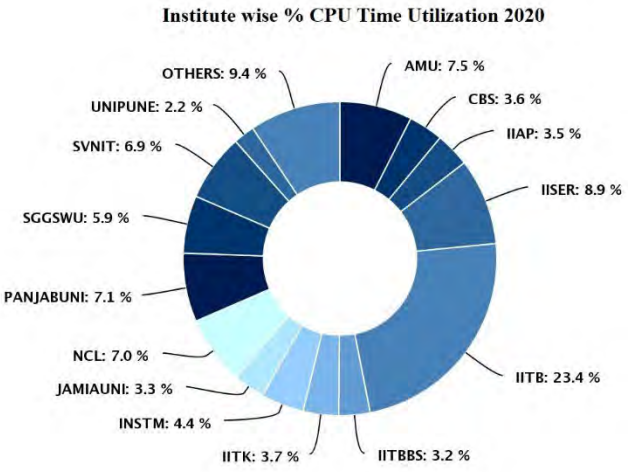


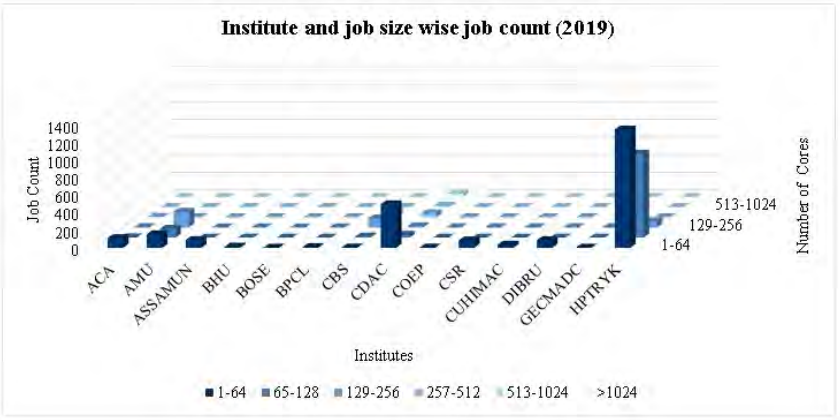
Table: Institute wise %CPU time utilization Year-2019

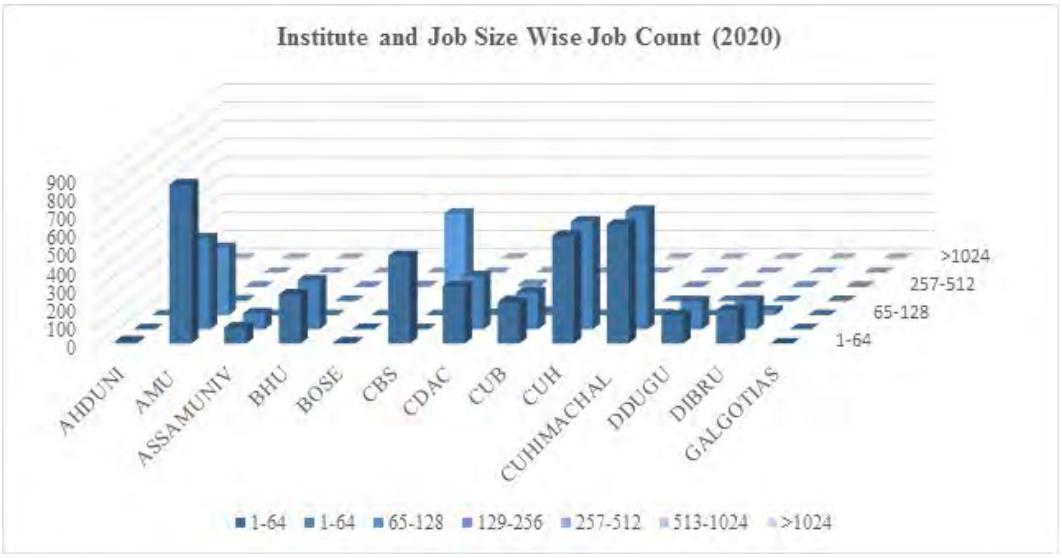
Institute	CPU Time Utilization(CPU seconds)
IITB	42850701633
IISERP	14594041136
SGGSWU	9317473024
IIAP	8249226240
PUCHD	5383295120
SVNIT	4760117152
IITK	4622852034
NCLPUNE	3946017617
IIITM	3818456813
CBS	3446545744
HPTRYK	3193726574
HPUNIV	3146808947
UNIPUNE	3034532016
OTHERS	12647639197

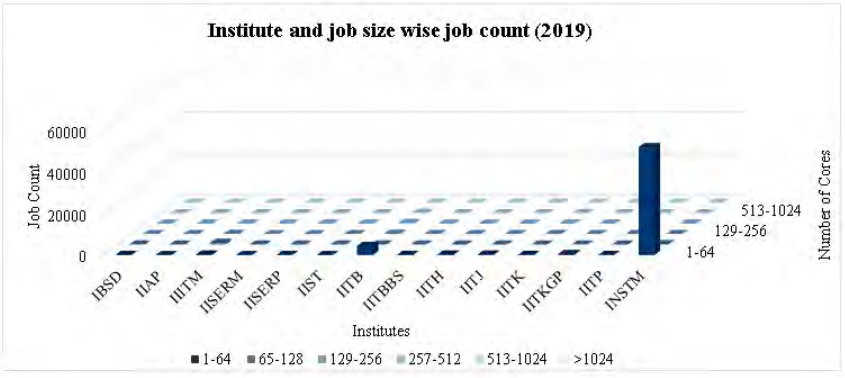
Table: Institute wise %CPU time utilization Year-2020

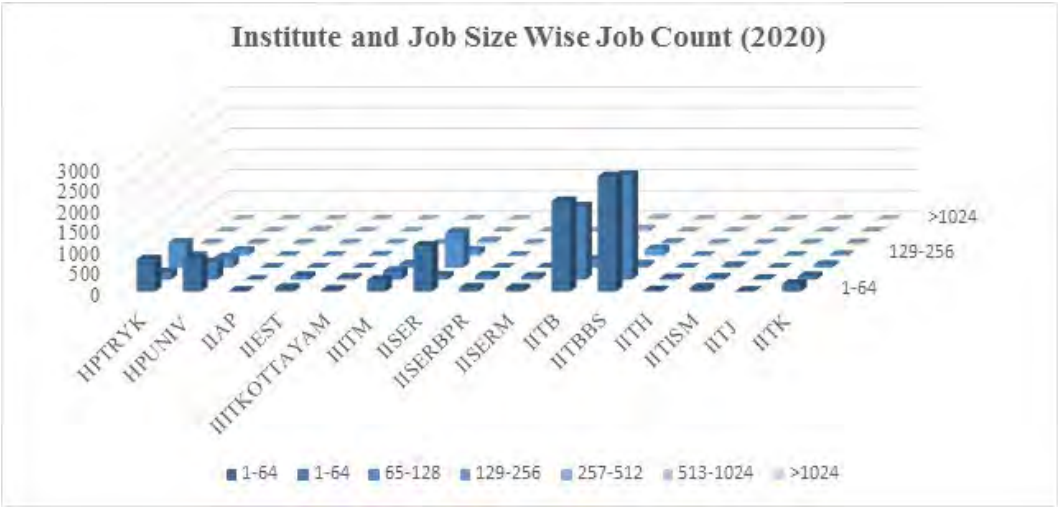
Institute	CPU Time Utilization(CPU seconds)
AMU	11680914652
CBS	5586661121
IIAP	5552407552
IISER	13974883722
IITB	36731751985
IITBBS	5022011785
IITK	5759608285
INSTM	6923370085
JAMIAUNI	5186984164
NCL	10917175882
PANJABUNI	11072784928
SGGSWU	9305446976
SVNIT	10843634994
UNIPUNE	3444399763
OTHERS	14707951743

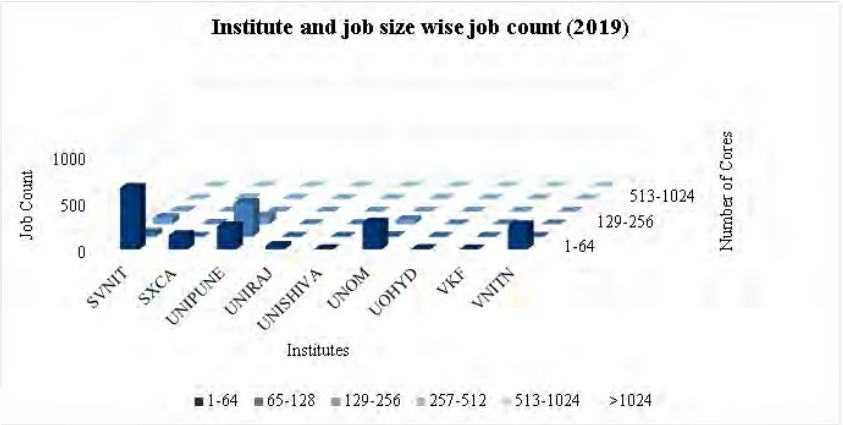
Institute and job size wise job count

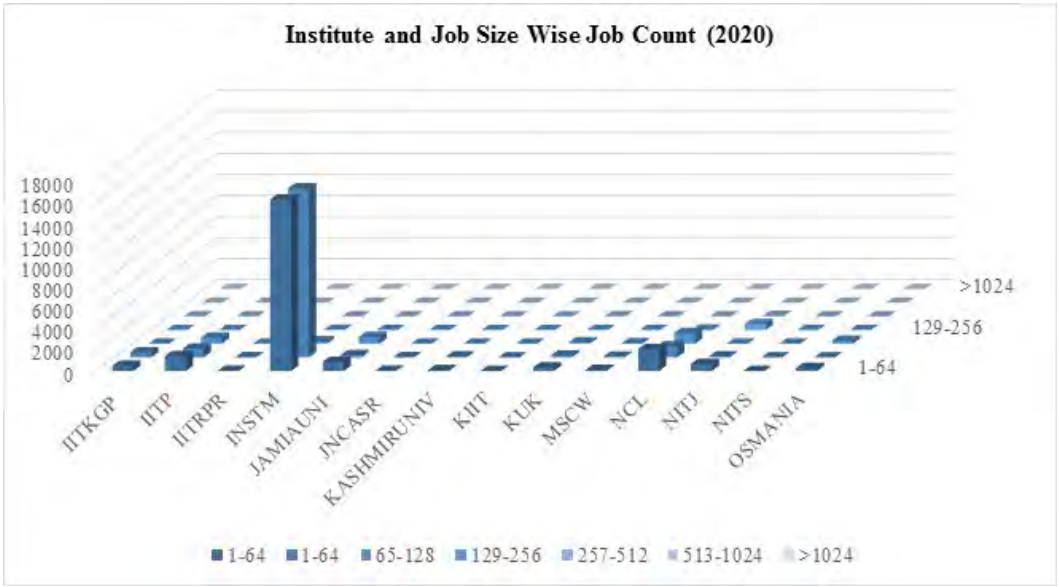







Institute and Job Size Wise Job Count (2020)
3000
2500
2000
1500
1000
500
0
>1024
129-256
1-64
IIPTRYK
HPUNIV
IIAP
IIEST
IIITKOTTAYAM
IIITM
IISER
IISERBPR
IISERM
IITB
IITBBS
IITH
IITISM
IITJ
IITK
1-64
1-64
65-128
129-256
257-512
513-1024
>1024


Institute and job size wise job count (2019)
Job Count
1000
500
0
513-1024
129-256
1-64
Number of Cores
SVNIT
SXCA
UNIPUNE
UNIRAJ
UNISHIVA
UNOM
UOHYD
VKF
VNITN
Institutes
1-64
65-128
129-256
257-512
513-1024
>1024


Institute and Job Size Wise Job Count (2020)
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
>1024
129-256
1-64
IITKGP
IITP
IITRPR
INSTM
JAMIAUNI
JNCASR
KASHMIRUNIV
KIIT
KUK
MSCW
NCL
NITJ
NITS
OSMANIA
1-64
1-64
65-128
129-256
257-512
513-1024
>1024

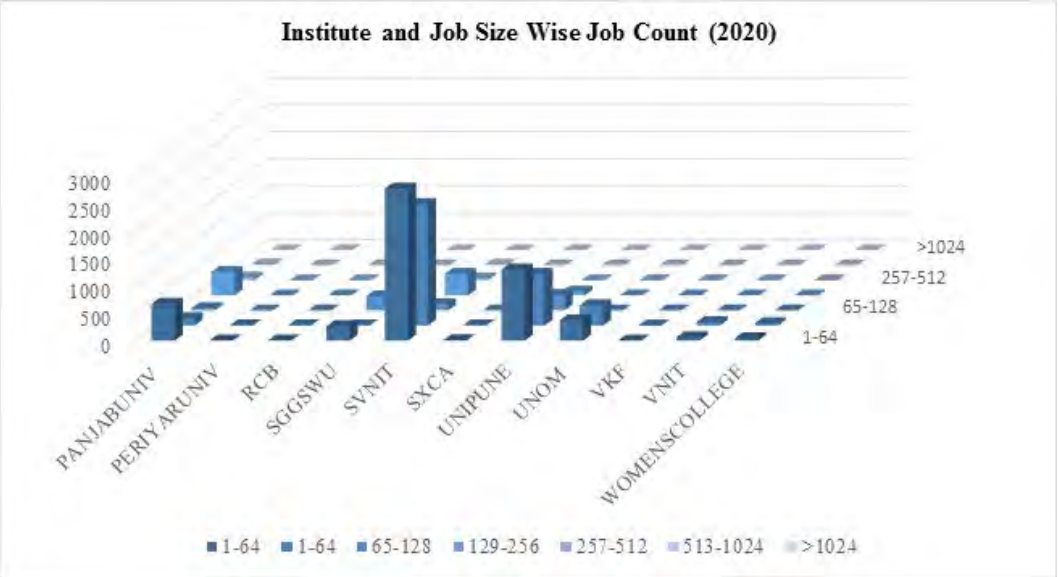


Table: Institute and Job size wise Job count Year – 2019

Institute	1-64	65-128	129-256	257-512	513-1024	>1024
ACA	109	3	2	5	0	0
AMU	153	99	177	2	0	0
ASSAMUNIV	88	0	0	0	0	0
BHU	12	0	0	0	0	0
BOSE	1	0	0	0	0	0
BPCL	8	0	0	0	0	0
CBS	2	11	101	83	0	0
CDAC	493	31	14	44	15	36
COEP	2	0	0	0	0	0
CSR	82	0	0	0	0	0
CUHIMACHALS	36	0	0	0	0	0
DIBRU	86	3	0	0	0	0
GECMADOSA	1	0	0	0	0	0
HPTRYK	1342	952	67	2	0	0
HPUNIV	583	641	277	35	21	0
IBSD	65	0	0	0	0	0
IIAP	0	0	0	0	25	2
IIITM	254	861	132	0	0	0
IISERB	4	0	0	0	0	0
IISERM	45	1	1	0	0	0
IISERP	479	778	164	56	0	0
IIST	2	0	0	0	0	0
IITB	4357	66	208	254	150	20

Institute	1-64	65-128	129-256	257-512	513-1024	>1024
IITBBS	148	12	50	1	0	0
IITH	223	0	0	0	0	0
IITJ	267	0	0	0	0	0
IITK	90	15	21	43	34	0
IITKGP	501	18	0	0	0	0
IITP	65	2	0	0	0	0
INSTM	51844	230	72	36	2	1
ISM	1	1	0	2	0	0
JMIUNIV	123	424	1	0	0	0
JNCASR	39	30	0	0	0	0
KUK	152	134	38	13	42	0
MSCW	67	0	0	0	0	0
NCLPUNE	1803	1693	45	0	0	0
OSMANIA	11	254	0	12	0	0
PONDIUNI	77	0	0	0	0	0
PUCHD	221	65	239	47	0	1
SASTRA	62	0	0	0	0	0
SGGSWU	2	223	15	0	0	0
SVNIT	660	40	68	8	0	0
SXCA	152	1	3	0	6	0
UNIPUNE	247	362	79	1	3	0
UNIRAJ	37	0	0	0	0	0
UNISHIVAJI	2	0	0	0	0	0
UNOM	289	8	0	0	2	0
UOHYD	3	0	0	0	0	0
VKF	1	0	0	0	0	0
VNITN	257	0	0	0	0	0

Table: Institute and Job size wise Job count Year – 2020

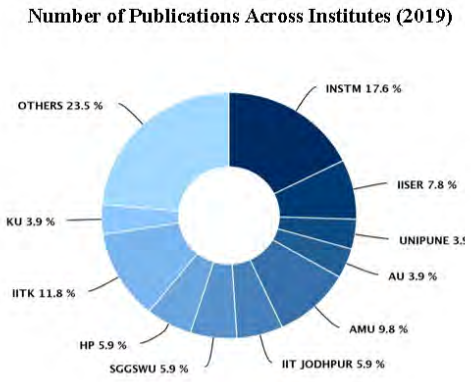
Institute	1-64	65-128	129-256	257-512	513-1024	>1024
AHDUNI	12	1	0	0	11	0
AMU	867	497	367	3	0	0
ASSAMUNIV	87	87	0	0	0	0
BHU	268	268	0	0	0	0
BOSE	5	3	0	0	2	0
CBS	478	1	0	476	1	0
CDAC	311	291	6	2	10	2
CUB	222	203	19	0	0	0

Institute	1-64	65-128	129-256	257-512	513-1024	>1024
CUH	588	588	0	0	0	0
CUHIMACHAL	649	646	3	0	0	0
DDUGU	154	154	0	0	0	0
DIBRU	182	157	25	0	0	0
GALGOTIAS	1	1	0	0	0	0
HPTRYK	783	181	602	0	0	0
HPUNIV	799	428	254	117	0	0
IIAP	26	0	0	0	0	26
IIEST	93	93	0	0	0	0
IIITKOTTAYAM	50	47	0	3	0	0
IIITM	287	207	80	0	0	0
IISER	1116	102	833	126	55	0
IISERBPR	100	100	0	0	0	0
IISERM	88	74	13	1	0	0
IITB	2187	1770	194	49	91	61
IITBBS	2785	2527	77	160	21	0
IITH	39	39	0	0	0	0
IITISM	99	53	43	2	1	0
IITJ	23	23	0	0	0	0
IITK	190	85	72	16	8	8
IITKGP	493	493	0	0	0	0
IITP	1415	835	580	0	0	0
IITRPR	18	17	1	0	0	0
INSTM	16302	16054	218	28	2	0
JAMIAUNI	870	225	643	2	0	0
JNCASR	18	8	0	9	1	0
KASHMIRUNIV	83	83	0	0	0	0
KIIT	2	2	0	0	0	0
KUK	339	182	134	10	13	0
MSCW	109	72	36	1	0	0
NCL	2094	1037	1013	41	3	0
NITJ	665	80	0	558	27	0
NITS	1	1	0	0	0	0
OSMANIA	295	2	281	12	0	0
PANJABUNIV	682	140	41	436	50	15
PERIYARUNIV	3	3	0	0	0	0

Institute	1-64	65-128	129-256	257-512	513-1024	>1024
RCB	4	4	0	0	0	0
SGGSWU	267	3	263	1	0	0
SVNIT	2812	2251	118	398	35	10
SXCA	7	6	1	0	0	0
UNIPUNE	1317	956	290	71	0	0
UNOM	378	378	0	0	0	0
VKF	1	1	0	0	0	0
VNIT	64	63	1	0	0	0
WOMENSCOLLEGE	45	45	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 2020 total of 67 Publications has been published using the PARAM Yuva II cluster.



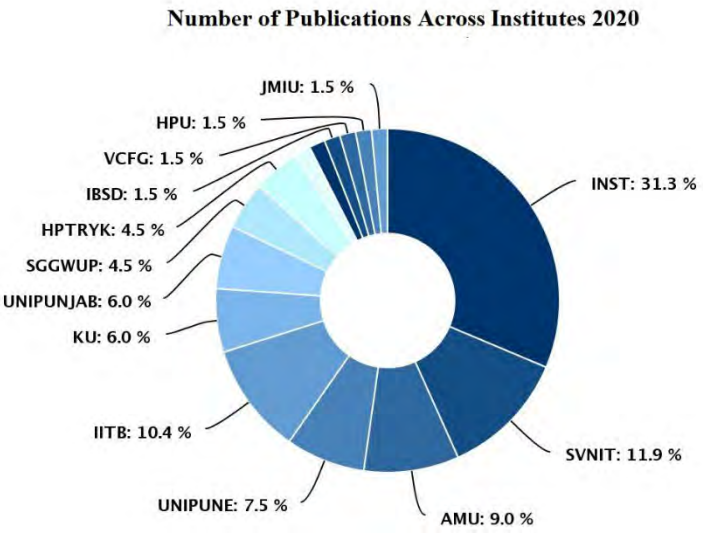


Table: Number of publications across institutes Year-2019

Institute	Number of Publications
INST Mohali	9
IISER	4
IIAP-Indian Institute of AstroPhysics	1
Unipune-Pune University	2
AssamUniv	2
AMU-Aligarh Muslim University	5

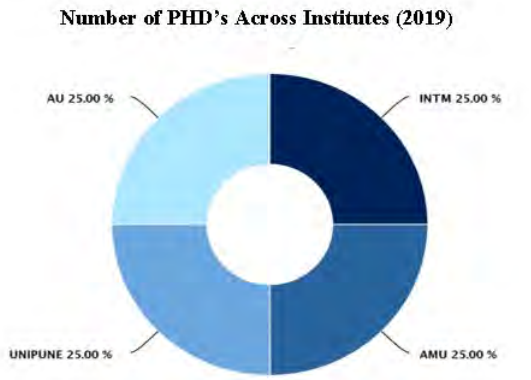
Institute	Number of Publications
IIT Guwhati	1
NCL Pune	1
IIT Jodhpur	3
SGGSWU	3
IPU- Indra Prasth University	1
HP university	3
IIT Kanpur	6
CBS Mumbai	1
Osmania Hyderabad	1
dibru- Dibrugarh University	1
GEC Madosa	1
JamiaUniv-Jamia Milia University	2
Kurukshetra University	3
Punjab University	2

Table: Number of publications across institutes Year-2020

Institute	Number of Publications
VKFG	1
INST Mohali	21
IBSD	1
IITB	7
IITH	1
IISER	1
Unipune-Pune University	5
JMIU	1
AMU-Aligarh Muslim University	6
SVNIT	8
SGGSWU	3
HP university	1
KU	4
HARSC	3
UNIPUNJAB	4

Number of Ph.D.'s across institutes

In 2020, eleven of the PARAM Yuva II Users have completed their Ph.D. and submitted their thesis, below are the details.



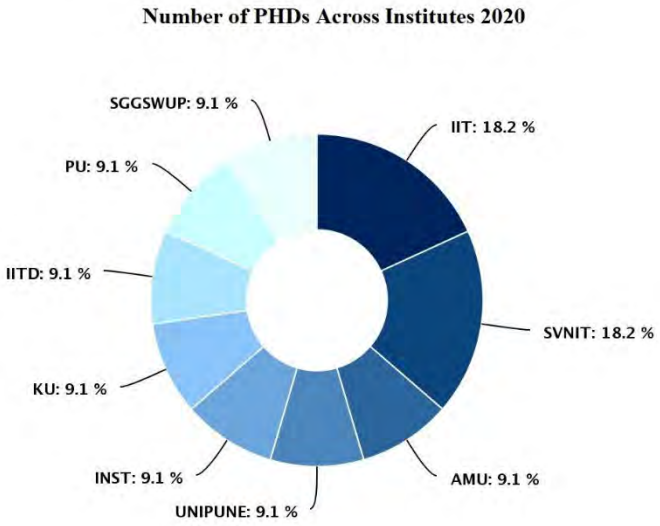


Table: Number of PhDs across institutes Year – 2019

Institute	Number of PhDs
INSTM	1
AMU	1
UNIPUNE	1
ASSAMUNIV	1

Table: Number of PhDs across institutes Year – 2020

Institute	Number of PhDs
AMU	1
IITB	2
IITD	1
INST	1
KU	1
PU	1
SGGSUF	1
SVNIT	2
UNIPUNE	1

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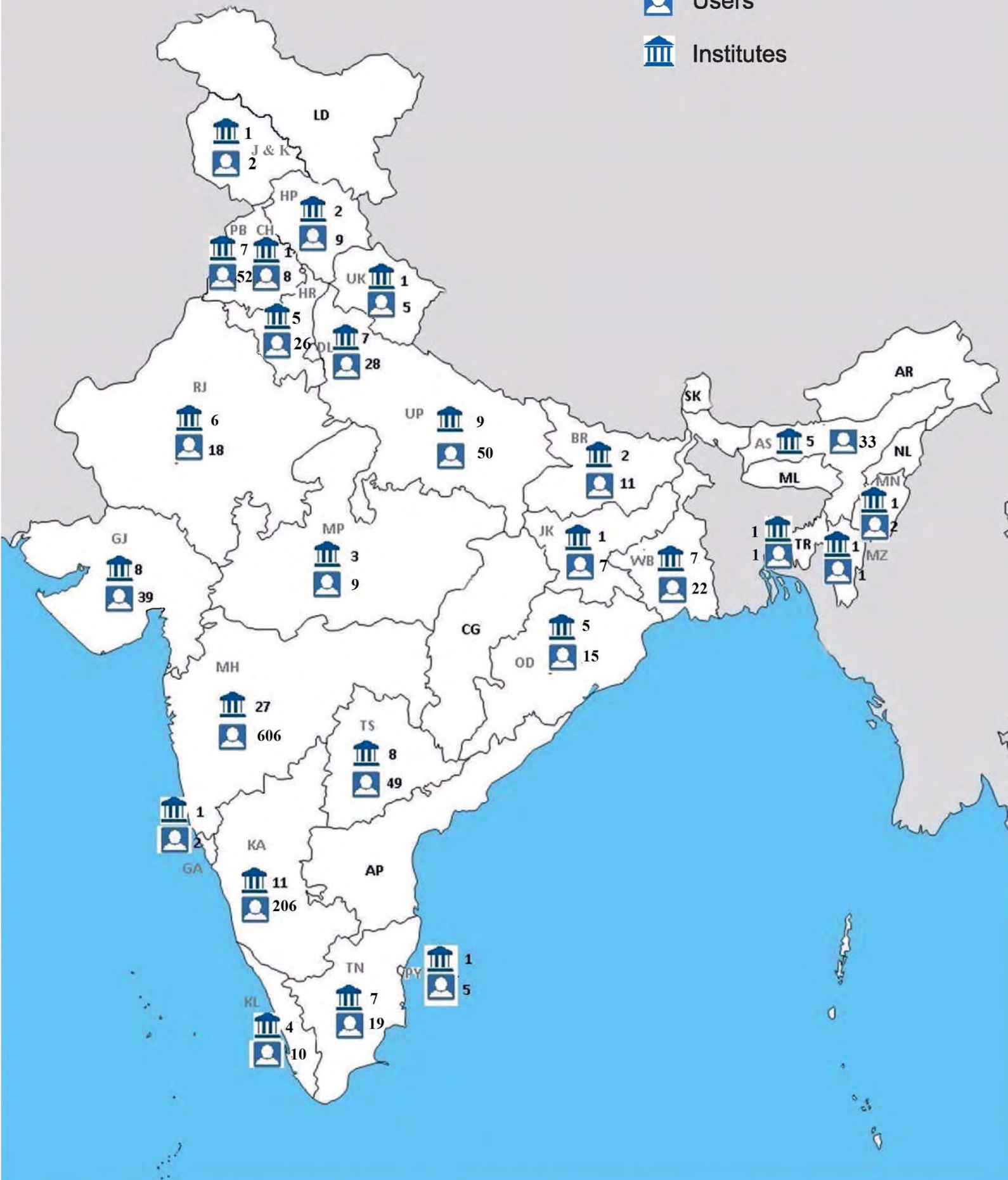
Table: State wise NPSF Users and Institutes

State or Union Territory	Short Name	No. of Institutions	No. of Users
Andhra Pradesh	AP	0	0
Arunachal Pradesh	AR	0	0
Assam	AS	5	33
Bihar	BR	2	11
Chandigarh	CH	1	8
Chhattisgarh	CG	0	0
National Capital Territory of Delhi	DL	7	28
Goa	GA	1	2
Gujarat	GJ	8	39
Haryana	HR	5	26
Himanchal Pradesh	HP	2	9
Jammu and Kashmir	J&K	1	2
Jharkhand	JK	1	7
Karnataka	KA	11	206
Kerala	KL	4	10
Ladakh	LD	0	0
Madhya Pradesh	MP	3	9
Maharashtra	MH	27	606
Manipur	MN	1	2
Meghalaya	ML	0	0
Mizoram	MZ	1	1
Nagaland	NL	0	0
Odisha	OD	5	15
Pondicherry	PY	1	5
Punjab	PB	7	52
Rajasthan	RJ	6	18
Sikkim	SK	0	0
Tamil Nadu	TN	7	19
Telangana	TS	8	49
Tripura	TR	1	1
Uttar Pradesh	UP	9	50
Uttarakhand	UK	1	5
West Bengal	WB	7	22

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.

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4.3 Research Field

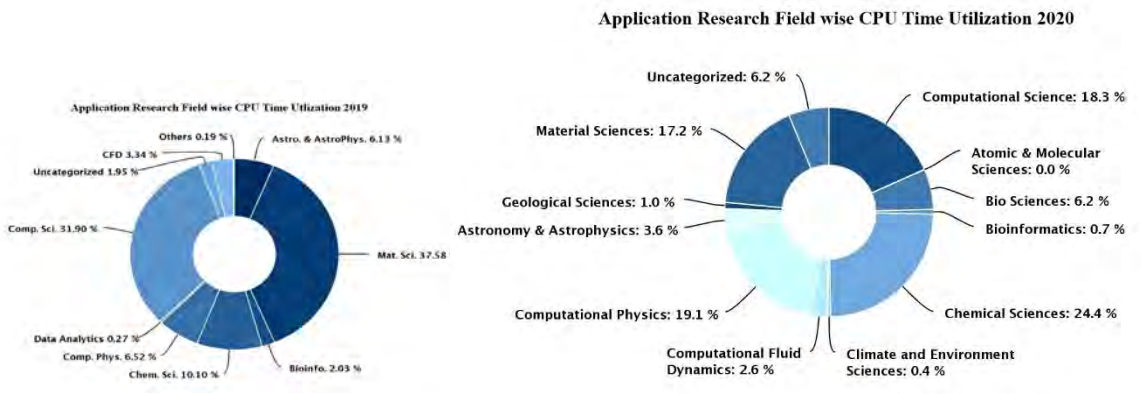
When affiliated with NPSF, users are classified according to their 1) Research Field and 2) Institute. Former is deduced from the area of work/application, whereas Institute is one of the attributes in the Technical Affiliation Scheme (TAS) form. This section presents CPU time distribution, job count, and job size distribution across various Research Fields and Institutes. The inferences that can be derived from this data are to assess and corroborate the percolation of HPC across application Research Fields and whether or not the usage is perpetual during the 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 Field
1	Astronomy & Astrophysics
2	Atomic & Molecular Sciences
3	Bio Sciences
4	Bioinformatics
5	Chemical Sciences
6	Climate & Environment Sciences
7	Complex Systems and Statistical Physics
8	Computational Fluid Dynamics
9	Computational Physics
10	Computational Sciences
11	Data analytics
12	Geological Sciences
13	Material Sciences
14	Structural Engineering Mechanics
15	Uncategorized

Research Field wise CPU time utilization

Below doughnut plot represents the % CPU time utilization by the jobs across application research fields. Material Science and Computational Science are the major contributors to the CPU time utilization and the Jobs count.

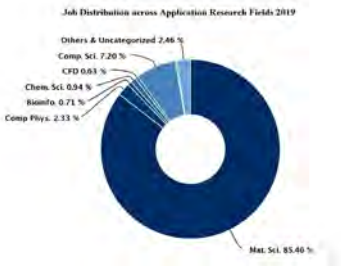


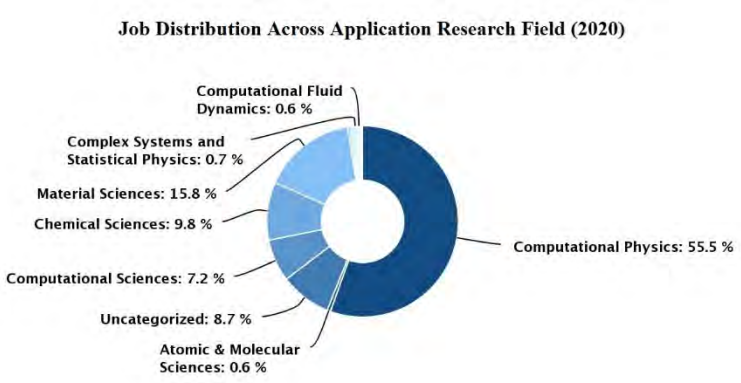
The above plots bring forth CPU time distribution across various application research fields.

Table: Research Field wise CPU time utilization

	CPU time in seconds	
Application Research Field	**2019**	**2020**
Astronomy and Astrophysics	8249226240	5552407552
Atomic & Molecular Sciences	615	69546775
Bio Sciences	1958586	9654114436
Bioinformatics	2731660017	1109614483
Chemical Sciences	13581185416	37888104207
Climate and Environment Sciences	379182337	648796608
Complex Systems and Statistical Physics	0	67135296
Computational Fluid Dynamics	4489924639	3994466286
Computational Physics	8768951681	29639336426
Computational Sciences	42908478613	28398418242
Data analytics	362913144	0
Geological Sciences	104204584	15426684008
Material Science	50551931751	26724497896
Quantum Mechanics	145360928	0
Structural Mechanics	0	0
Uncategorized	2622816306	9682392056

Job distribution across application research fields



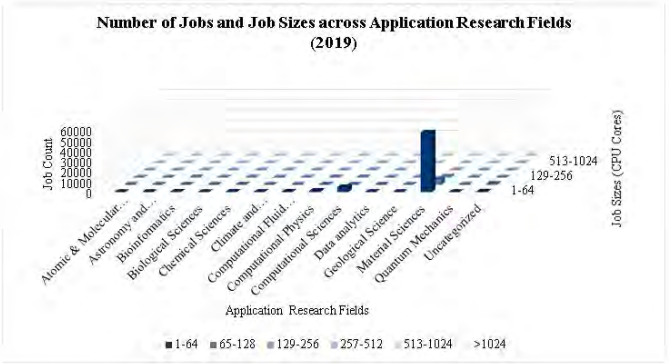


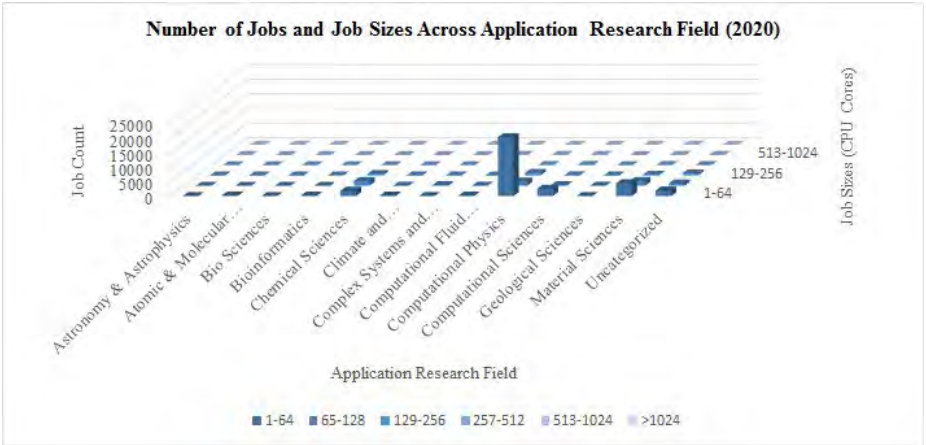
The above plots show application research fields-wise percentage distribution of the number of jobs processed.

Table: Job distribution across application research fields

	No. of Jobs	
Application Research Field	**Job Count 2019**	**Job Count 2020**
Atomic & Molecular Sciences	10	238
Astronomy and Astrophysics	27	26
Bioinformatics	537	191
Biological Sciences	67	36
Chemical Science	706	3994
Climate and Environment Sciences	143	182
Computational Fluid Dynamics	473	232
Complex systems & statistical physics	0	295
Computational Physics	1752	22613
Computational Science	5417	2918
Data analytics	207	0
Geological Science	4	68
Material Science	64340	6451
Quantum Mechanics	69	0
Uncategorized	1532	3529

Job sizes across application research fields





The above plots depict the distribution of jobs in reference to the 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 2019

Application Research Fields	**1-64**	**65-128**	**129-256**	**257-512**	**513-1024**	**>1024**
Atomic & Molecular Sciences	10	0	0	0	0	0
Astronomy and Astrophysics	0	0	0	0	25	0
Bioinformatics	212	101	177	8	6	33
Biological Sciences	67	0	0	0	0	0
Chemical Sciences	273	3	0	83	0	0
Climate and Environment Sci-	102	3	0	38	0	0
Computational Fluid Dynamics	360	15	21	43	34	0
Computational Physics	1173	199	277	60	42	1
Computational Sciences	4709	74	208	254	152	20
Data analytics	152	29	14	0	9	3
Geological Science	1	1	0	2	0	0
Material Sciences	57941	5308	908	150	32	1
Quantum Mechanics	67	2	0	0	0	0
Uncategorized	481	992	53	6	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	0	0	0
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 and 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						
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 the Application Research field. The majority of the Publications belong to the Material Science domain.

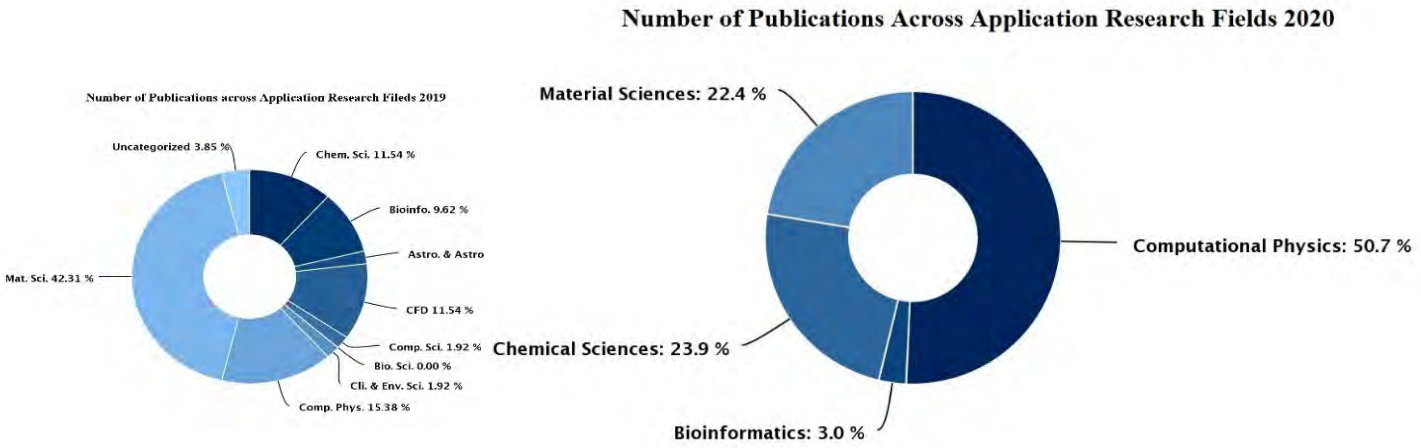
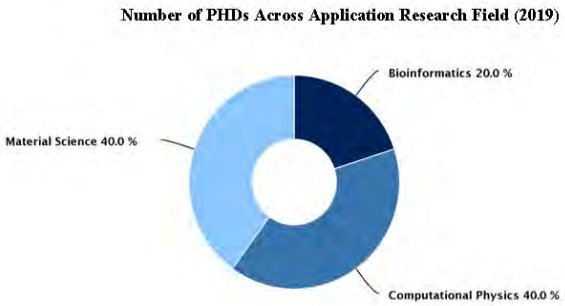


Table: Number of publications across research fields

	Number of Publications	
Application Research Fields	**Publication Count 2019**	**Publication Count 2020**
Astronomy & Astrophysics	1	0
Atomic and Molecular Science	0	0
Bioinformatics	5	2
Bio Science	0	0
Chemical Science	6	16
Climate & Environmental Science	1	0
Complex Systems & Statstical Physics	0	0
Computational Fluid Dynamics	6	0
Computational Physics	8	34
Computational Science	1	0
Geological Science	0	0
Material Science	22	15
Uncategorized	2	0

Number of PhDs across research fields



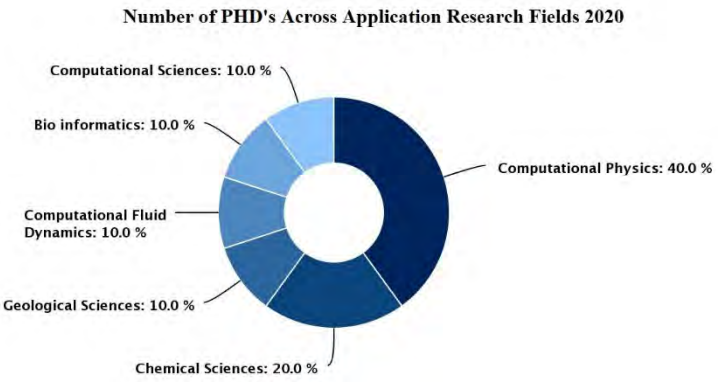


Table: Number of PhDs across research fields

	Number of PhDs	
Application Research Fields	**Number of PhDs 2019**	**Number of PhDs 2020**
Bio Science	0	0
Chemical Science	0	2
Bioinformatics	1	1
Computational Science	0	1
Material Science	2	1
Climate & Environmental Science	0	0
Computational Physics	1	4
Geological Sciences	0	1
Computational Fluid Dynamics	0	1

4.4 Ph.D. Theses

Title of the thesis: Studies on Protein Folding and Aggregation
Ph.D. Scholar Name: Ishrat Jahan
Name of the Supervisor: Prof. Md. Shahid Nayeem
Name of the Insititute: Aligarh Muslim University

Title of the thesis: 3D Inversion of Magnetotelluric Data over Dalma Volcano-Sedimentary, Dhanjori Volcanics and Bakreshwar Geothermal Province, Eastern Indian Shield
Ph.D. Scholar Name: Roshan Kumar Singh
Name of the Supervisor: Prof. Shalivahan
Name of the Institute: Indian Institute of Technology, Dhanbad

Title of the thesis: Renewable Energy Resources
Ph.D. Scholar Name: Vikram
Name of the Supervisor: Prof. Aftab Alam
Name of the Institute: Indian Institute of Technology, Bombay.

Title of the thesis: Development of a Novel Accurate VOF method for Incompressible Two-Phase Fluid Flow
Ph.D. Scholar Name: Sourabh Pramod Bhat
Name of the Supervisor: Prof. J. C. Mendal
Name of the Institute: Indian Institute of Technology, Bombay.

Title of the thesis: Ab-intio Study of some Silicon-Based 2D Materials for Energy and Sensing Applications.
Ph.D. Scholar Name: Radha N Somaiya
Name of the Supervisor: Dr. Yogesh Sonvane
Name of the Institute: Sardar Vallabhbhai National Institute of Technology, Surat.

Title of the thesis: Design and Synthesis of Small Molecule for Amyloid-β (Aβ) Aggregation in Alzheimer's Disease.
Ph.D. Scholar Name: Amandeep Kaur
Name of the Supervisor: Dr. Deepti Goyal
Name of the Institute: Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab.

Title of the thesis: Morphological and Thermophysical Properties of Metal-Oxide Nanofluids.
Ph.D. Scholar Name: Jankis Shah
Name of the Supervisor: Dr. Yogesh Sonvane
Name of the Institute: Sardar Vallabhbhai National Institute of Technology, Surat.

Title of the thesis: Exploring Half-Heusler Compounds for Thermoelectric Applications
Ph.D. Scholar Name: Anuradha
Name of the Supervisor: Prof. Ranjan Kumar, Dr. Ranber Singh
Name of the Institute: Punjab University, Chandigarh.

Title of the thesis: Computational Studies on Adrenergic GPCR
Ph.D. Scholar Name: Shruti Koulgi
Name of the Supervisor: Dr. Manali Joshi
Name of the Institute: Centre for Development of Advanced Computing, Pune

Title of the thesis: 2D transition-metal Dichalcogenide Monolayers and their Janus structures for next-generation electronics and energy conversion: an Ab-initio study
Ph.D. Scholar Name : Nityasagar Jena
Name of the Supervisor: Prof. Abir De Sarkar
Name of the Institute: Institute of Nano Science and Technology, Mohali

Title of the thesis: Magnetic Properties of Novel Rare Earth Free Permanent Magnet Materials
Ph.D. Scholar Name: Priti Rani
Name of the Supervisor: Dr. Manish K. Kashyap
Name of the Institute: Kurukshetra University, Kurukshetra

4.5 Publications

Publications by NPSF users

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

Following publications resulted from NPSF usage by its user. The publications are listed by the impact factors of the journal they are published in. The impact factor (IF) of an academic journal reflects the average number of citations to recent articles published in the journal.

Publications 2020

Chemical Reviews (53.904)

Jijun Zhao, Qiuying Du, Si Zhou,* and Vijay Kumar*, "Endohedrally Doped Cage Clusters" chem. Rev. 2020, 120, 17, 9021–9163

Journal of Materials Chemistry A (11.301)

Taniya Purkait, Dimple, Navpreet Kamboj, Manisha Das, Subhajit Sarkar, Abir De Sarkar, Ramendra Sundar Dey, "Electrochemically customized assembly of hybrid xerogel material via combined covalent and non-covalent conjugation chemistry: An approach for boosting the cycling performance of pseudocapacitors" Journal of Materials Chemistry A, 8(2020) 6740-6756

Soumi Haldar, Achintya Kumar Dutta, "A Multilayer Approach to the Equation of Motion Coupled-ClusterMethod for the Electron Affinity", J. Phys. Chem. A, 124, 3947−3962 (2020)

ACS Applied Materials & Interfaces (8.758)

Manish Kumar Mohanta, Abir De Sarkar, "Tweaking the Physics of Interfaces between Monolayers of Buckled Cadmium Sulfide for a Superhigh Piezoelectricity, Excitonic Solar Cell Efficiency, and Thermoelectricity", ACS Appl. Mater. Interfaces 2020, 12 (15), 18123–18137.

Manish Kumar Mohanta, Ashima Rawat, Nityasagar Jena, Dimple, Raihan Ahammed, Abir De Sarkar, "Interfacing Boron Monophosphide with Molybdenum Disulfide for an Ultrahigh Performance in Thermoelectrics, Two-Dimensional Excitonic Solar Cells, and Nanopiezotronics", ACS Appl. Mater. Interfaces 2020, 12 (2), 3114–3126.

Harpreet Singh, Manisha Devi, Nityasagar Jena, Mohamed Musthafa Iqbal, Yogendra Nailwal, Abir De Sarkar*, Santanu Kumar Pal*, "Proton Triggered Fluorescence Switching in Self-Exfoliated Ionic Covalent Organic Nanosheets for Applications in Selective Detection of Anions", ACS Applied Materials & Interfaces12 (2020) 13248-13255.

Nanoscale (6.895)

Manish Kumar Mohanta and Abir De Sarkar*, “Interfacial hybridization of Janus MoSSe and BX (X= P, As) monolayers for ultrathin excitonic solar cell, nanopiezotronics, and low-power memory devices”, Nanoscale 12 (2020) 22645-22657

Applied Surface Science (6.182)

Manish Kumar Mohanta, Abir De Sarkar*,"Giant tunability in electrical contacts and doping via inconsiderable normal electric field strength or gating for a high-performance in ultrathin field effect transistors based on 2D BX/graphene (X = P, As) van der Waals heterobilayer" Applied Surface Science, 526 (2020) 146749.

Taniya Purkait, Raihan Ahammed, Abir De Sarkar, Ramendra Sundar Dey, "The role of exfoliating solvents for control synthesis of few-layer graphene-like nanosheets in energy storage applications: Theoretical and experimental investigation", Applied Surface Science 509 (2020) 145375

Raihan Ahammed, Ashima Rawat, Nityasagar Jena, Dimple, Manish Kumar Mohanta, Abir De Sarkar*,"ZrS3/MS2 and ZrS3/MXY (M=Mo, W; X, Y=S, Se, Te; X ≠ Y) type-II van der Waals hetero-bilayers: Prospective candidates in 2D excitonic solar cells", Applied Surface Science, 499 (2020)143894.
Manish Kumar Mohanta, Abir De Sarkar, "2D HfN2/Graphene Interface Based Schottky Device: Unmatched Controllability in Electrical Contacts and Carrier Concentration via Electrostatic Gating and out-of-Plane Strain", Applied Surface Science 2020, 540, 148389.

Shagun Nag, Anuradha Saini, Ranber Singh, Ranjan Kumar, "Ultralow lattice thermal conductivity and anisotropic thermoelectric performance of AA stacked SnSe bilayer", Appl. Surf. Sci., 512, 145640 (2020)
V. Kumar, K. Rajput and D. R. Roy*, "Monolayer Bi2C3: A promising sensor for environmentally toxic NCGs with high sensitivity and selectivity", Applied Surf. Sci. (Elsevier Sci) 534 (2020) 147609.DOI: 10.1016/j.apsusc.2020.147609

K. Rajput, V. Kumar and D. R. Roy*, "Heterobilayer CaS/CaSe: A promising sensor for environmental toxic NO2 gas with high selectivity and sensitivity", Applied Surf. Sci. (Elsevier Sci) 528 (2020) 146996.DOI: 10.1016/j.apsusc.2020.146996

Journal of CO2 Utilization (5.993)

SS Deshpande, MD Deshpande, T Hussain, R Ahuja, "Investigating CO2 storage properties of C2N monolayer functionalized with small metal clusters", Journal of CO2 Utilization 35, 1-13 (2020).

Materials Science and Engineering B (5.88)

Pooja Kapoor, Ashok Kumar, P. K. Ahluwalia, Size-dependent electronic, mechanical and optical properties of noble metal nanoribbons, December 2020, Materials Science and Engineering B 262(4):114786, DOI: 10.1016/j.mseb.2020.114786

Catalysis Today (5.825)

Mondal, Unmesh, and Prasenjit Ghosh. "Role of geometry, charge and fluxionality of clusters in CO2 activation on supported sub-nanometer metal clusters: The case of Cu tetramers on pristine and O-terminated MXene." Catalysis Today (2020) DOI: 10.1016/j.cattod.2020.09.002

International Journal of Biological Macromolecules (5.162)

Imrat , Rajendra Kumar Labala , Shilpa Velhal , Sharad Bhagat , Vainav Patel , Kumaraswamy Jeyaram "Small double-stranded RNA with anti-HIV activity abundantly produced by Bacillus subtilis MTCC5480 isolated from fermented soybean",DOI: 10.1016/j.ijbiomac.2020.06.112

Journal of Molecular Liquids (5.065)

Faisal Ameen, Sharmin Siddiqui, Ishrat Jahan, Shahid M.Nayeem, Sayeed ur Rehman, Mohammad Tabish, "A

detailed insight into the interaction of memantine with bovine serum albumin: A spectroscopic and computational approach", Journal of Molecular Liquids, Volume 303, 112671 (2020)

Journal of Chemical Theory and Computation (5.011)

Madhubani Mukherjee, Divya Tripathi, Martin Brehm, Christoph Riplinger, Achintya Kumar Dutta, "Efficient EOM-CC-based Protocol for the Calculation of Electron Affinity of Solvated Nucleobases: Uracil as a Case Study", J. Chem. Theory & Comput., 17, 1, 105–116

The FEBS Journal (4.739)

Nikunj Raninga, Shahid M. Nayeem, Sowmiya Gupta, Ranajoy Mullick, Esha Pandita, aumitra Das, Shashank Deep, Apurba Kumar Sau, " Stimulation of GMP formation in hGBP1 is mediated by W79 and its effect on the antiviral activity", The FEBS J, https://doi.org/10.1111/febs.15611 (2020)

Journal of Alloys and Compounds (4.650)

Priti Rani, Manish K Kashyap, Renu Singla, Jyoti Thakur, Ali H Reshak, "Magnetism and magnetocrystalline anisotropy of tetragonally distorted L10-FeNi: N alloy", Journal of Alloys and Compounds, 835, 155325, 2020.

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M. S. Bhadane, K. H. Gavhane, V. S. Ghemud, S. S. Dahiwale, P. S. Patil, Anjali Kshirsagar and S. D. Dhole, “A post annealing effect on SrF2 nano particles: Structural, morphological, functional and dosimetric properties”, 156343 (2020)

Renu Singla, Sarvesh Kumar, Timothy A Hackett, Ali H Reshak, Manish K Kashyap, "Genesis of magnetism in graphene/MoS2 van der Waals heterostructures via interface engineering using Cr-adsorption", Journal of Alloys and Compounds, 859, 157776

Anuradha Saini, Shagun Nag, Ranber Singh, Ranjan Kumar, "Unraveling the effect of isotropic strain on the transport properties of half-Heusler alloy LiScGe", J. Alloys Compd, 859, 158232

ACS Applied Energy Materials (4.473)

Sachin R. Rondiya, Yogesh Jadhav, Nelson Y. Dzade, Raihan Ahammed, Tanmay Goswami, Abir De Sarkar, Sandesh Jadkar, Santosh K. Haram, Hirendra N. Ghosh, “An Experimental and Theoretical Study into Interface Structure and Band Alignment of the Cu2Zn1-xCdxSnS4 Heterointerface for Photovoltaic Applications”, ACS Applied Energy Materials, 3(6) (2020) 5153–5162

Journal of Physical Chemistry C. (4.189)

Raihan Ahammed, Nityasagar Jena, Ashima Rawat, Manish Kumar Mohanta, Dimple and Abir De Sarkar*,“Ultrahigh Out-of-Plane Piezoelectricity Meets Giant Rashba Effect in 2D Janus Monolayers and Bilayers of Group IV Transition Metal Trichalcogenides”, J. Phys. Chem. C, 124 (39) (2020) 21250-21260

Ashima Rawat, Manish Kumar Mohanta, Nityasagar Jena, Dimple, Raihan Ahammed, Abir De Sarkar*, “Nanoscale Interfaces of Janus Monolayers of Transition Metal Dichalcogenides for 2D Photovoltaic and Piezoelectric Applications”, Journal of Physical Chemistry C 124 (2020) 10385–10397.

Anusri Medda, Avisek Dutta, Dipankar Bain, Manish Kumar Mohanta, Abir De Sarkar*, Amitava

Patra*,“Electronic Structure Modulation of 2D Colloidal CdSe Nanoplatelets by Au25 Clusters for High-Performance Photodetector”, J. Phys. Chem. C 124 (2020)19793–19801

Avisek Dutta, Anusri Medda, Rajesh Bera, Ashima Rawat, Abir De Sarkar*, Amitava Patra*, "Electronic Band Structure and Ultrafast Carrier Dynamics of Two Dimensional (2D) Semiconductor Nanoplatelets (NPLs) in the Presence of Electron Acceptor for Optoelectronic Applications", J. Phys. Chem. C 124 (2020) 26434–26442

Physical Review B (3.575)

Manish Kumar Mohanta, Abir De Sarkar, "Coupled Spin and Valley Polarization in Monolayer HfN2 and Valley-Contrasting Physics at the HfN2-WSe2 Interface", Phys. Rev. B 2020, 102 (12), 125414.

Physica E: Low-dimensional systems and nanostructures (3.570)

Manish Kumar Mohanta, Dimple, Ashima Rawat, Nityasagar Jena, Raihan Ahammed, Abir De Sarkar, "Ultra-Low Thermal Conductivity and Super-Slow Hot-Carrier Thermalization Induced by a Huge Phononic Gap in Multifunctional Nanoscale Boron Pnictides", Physica E: Low-dimensional Systems and Nanostructures 2020, 124, 114222.

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K. Rajput and D. R. Roy*, "Hybrid CaS/CaSe bilayer as a wide temperature range thermoelectric material", Physica E (Elsevier Science) 119 (2020) 114014(1-8). DOI: 10.1016/j.physe.2020.114014

Nanotechnology (3.551)

Rajesh Thakur, P K Ahluwalia, Ashok Kumar, and Raman Sharma, "Strain modulated carrier mobility and optical properties of graphene nanowiggles", Nanotechnology 31 (2020) 505202

Manish Kumar Mohanta, Amal Kishore, Abir De Sarkar*, "Two-dimensional ultrathin van der Waals heterostructures of indium selenide and boron monophosphide for superfast nanoelectronics, excitonic solar cells, and digital data storage devices", Nanotechnology 31(2020) 495208

Journal of Biomolecular Structure and Dynamics (3.549)

Faisal Ameen, Sharmin Siddiqui, Tasneem Kausar, Shahid M. Nayeem, Tarique Sarwar, Mohammad Moshahid Alam Rizvi, Sayeed Rehman & Mohammad Tabish, "Interaction of memantine with calf thymus DNA: an in-vitro and in-silico approach and cytotoxic effect on the cancerous cell lines", JBSD,1823886 (2020)

Physical Chemistry Chemical Physics (3.430)

Raquel Esteban-Puyuelo, Rajat Kumar Sonkar, Bhalchandra Pujari, Oscar Grånas, and Biplab Sanyal, "Tailoring the optoelectronic response of graphene nanoflakes by size and shape optimization", Phys.Chem.Chem.P, 22,8212, (2020)

Anupamjeet Kaur, Suniba Shuaib, Deepti Goyal, Bhupesh Goyal, “Interactions of a multifunctional di-triazole derivative with Alzheimer's Aβ42 monomer and Aβ42 protofibril: a systematic molecular dynamics study”, Physical Chemistry Chemical Physics, 22, 1543–1556 (2020).

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Manish Kumar Mohanta, Fathima IS, Abir De Sarkar*, "Exceptional mechano-electronic properties in HfN2 monolayer: promising candidate in low-power flexible electronics, memory devices and photocatalysis" Physical Chemistry Chemical Physics, 22(2020) 21275-21287

K. Rajput and D. R. Roy*, "2D PC3 as a promising thermoelectric material", Phys. Chem. Chem. Phys. (Royal Soc. Chem.) 22 (2020) 8625-8632.DOI: 10.1039/D0CP00527D

Materials Chemistry and Physics (3.408)

Namrata Jaykhedkar, Nilakantha Tripathy, Vaishali Shah, Bhalchandra Pujari, S. Premkumar, "A comprehensive study of pressure dependent phase transitions in ferroelectric PbTiO3 , PbZrO3 and BaTiO3" Materials Chemistry and Physics 254, 123545 (2020)

ChemPhysChem (3.144)

Santosh Ranga, Madhubani Mukherjee, Achintya Kumar Dutta, "Interactions of Solvated Electrons with Nucleobases: The Effect of Base Pairing", ChemPhysChem, 21, 1019–1027 (2020)

RSC Advances (3.119)

Ishrat Jahan, Shahid M. Nayeem, " Conformational dynamics of superoxide dismutase (SOD1) in osmolytes: a molecular dynamics simulation study", RSC Adv., 10, 27598-27614 (2020)

Journal of Chemical Physics (2.99)

Madhubani Mukherjee, Divya Tripathi, Achintya Kumar Dutta, "Water mediated electron attachment to nucleobases: Surface-bound vs bulk solvated electrons", J. Chem. Phys. 153, 044305 (2020)

Vacuum (2.906)

Renu Singla, Jyoti Thakur, Priti Rani, Sarvesh Kumar, Timothy A Hackett, Manish K Kashyap, "Emergence of magnetic behavior in AB-stacked bilayer graphene via Fe-doping", Vacuum, 182, 109685, 2020.

ACS Omega (2.87)

Amandeep Kaur, Anupamjeet Kaur, Deepti Goyal, Bhupesh Goyal, “How does the mono-triazole derivative modulate Aβ42 aggregation and disrupt a protofibril structure: insights from molecular dynamics simulations”, ACS Omega, 5, 15606–15619 (2020).

Ashma Khan, Shahid M. Nayeem, "Effect of TMAO and Urea on Dimers and Tetramers of Amyloidogenic Heptapeptides (23FGAILSS29)", ACS Omega, 5, 42, 26986–26998 (2020)

Journal of Physics: Condensed Matter (2.707)

Deepashri Saraf and Anjali Kshirsagar*, “Theoretical prediction of stable cluster-assembled CdSe bilayer and its functionalization with Co and Cr adatoms”, DOI: 10.1088/1361-648X/ab432732, Journal of Physics: Condensed Matter

Dimple, Manish Kumar Mohanta, Ashima Rawat, Nityasagar Jena, Raihan Ahammed, Abir De Sarkar*, “Ultra-low lattice thermal conductivity and giant phonon-electric field coupling in hafnium dichalcogenide monolayers”, Journal of Physics: Condensed Matter 32 (2020) 315301

Manish Kumar Mohanta, Ashima Rawat, Nityasagar Jena, Raihan Ahammed, Abir De Sarkar, "Superhigh Flexibility and Out-of-Plane Piezoelectricity Together with Strong Anharmonic Phonon Scattering Induced

Extremely Low Lattice Thermal Conductivity in Hexagonal Buckled CdX (X = S, Se) Monolayers", Journal of Physics: Condensed Matter 2020, 32 (35), 355301.

Solid State Sciences (2.434)

P Rambabu, B Anuroopa, M. Manivel Raja, V. Kanchana, "Enhanced Curie temperature and spin polarization in Co-based compounds under pressure: A first principles investigation", Solid State Sciences, 105, 106257 (2020)

Journal of Applied Physics (2.286)

Renu Rani, Nityasagar Jena, Anirban Kundu, Abir De Sarkar*, Kiran Shankar Hazra*, "Impact of transverse and vertical gate electric field on vibrational and electronic properties of MoS2", Journal of Applied Physics, 127 (2020) 145101.

SR Kumavat, Y Sonvane, SK Gupta, Structural, optical, transport, and solar cell properties of 2D halide perovskite MAZX3 (Z = Pb, Sn, and X = Cl, Br, I), Journal of Applied Physics 128 (11), 114304

Journal of Molecular Graphics and Modelling (2.079)

SY Wakhare, MD Deshpande, "Structural, electronic and optical properties of metalloid element (B, Si, Ge, As, Sb, and Te) doped g-ZnO monolayer: A DFT study", Journal of Molecular Graphics and Modelling, 101, 107753-107762, (2020).

Swapnil S Deshpande, Dipali B Potekar, P B Shelake, MD Deshpande, "Theoretical study of interaction of Fe13O8@ Zn48O48 cluster with dopamine: Magnetic and optical properties", Journal of Molecular Graphics and Modelling, 107640-107650, (2020).

Naunyn-Schmiedeberg's Archives of Pharmacology (2.05)

Sumayya Shahzad, Somaiya Mateen, Tasneem Kausar, Syed Shariq Naeem, Asif Hasan, Minhal Abidi, Shahid M. Nayeem, Abul Faiz Faizy & Shagufta Moin, " Effect of syringic acid and syringaldehyde on oxidative stress and inflammatory status in peripheral blood mononuclear cells from patients of myocardial infarction", Naunyn-Schmiedeberg's Archives of Pharmacology volume 393, 691–704(2020)

Chemical Physics (1.771)

Santosh Ranga, Achintya Kumar Dutta, "A Core-Valence Separated Similarity Transformed EOM-CCSD Method for Core-excitation Spectra",Chemical Physics, arXivpreprint arXiv:2010.08932,

Pooja Verma, Debashree Ghosh, Achintya Kumar Dutta, "Electron attachment to Cytosine: The Role of Water", Chemical Physics, arXiv: 2010.14888v2

International Journal of Quantum Chemistry (1.747)

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P. Kumar, K. Rajput and D. R. Roy*, "DFT investigation on the optical properties of 2D-CaSe", AIP Conf. Proc. 2265 (2020) 030496. DOI: 10.1063/5.0017554

K. Rajput and D. R. Roy*, "Thermoelectric investigation on Mg3N2 monolayer", AIP Conf. Proc. 2265 (2020) 030640. DOI: 10.1063/5.0017733

P. Kumar, K. Rajput and D. R. Roy*, "First principle investigation on the optical properties of monolayer CaS", AIP Conf. Proc. 2220 (2020) 130070. DOI: 10.1063/5.0001254

K. Rajput and D. R. Roy*, "Investigation on the thermoelectric properties of single & bilayers of SrS", AIP Conf. Proc. 2220 (2020) 130071. DOI: 10.1063/5.0001255

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5. Visits

Total number of visits by dignitaries during Year-2020: 5

5.1 Visits by Dignitaries

- Dr. Santosh Kumar Pandey, Sc.D/Joint Director, Meity, Delhi
- Mr. Pankaj Mishra, Survey of India, Dehradun
- Dy. Comdt AS Rathi, MTI(IMD)
- Mr. Sanjit Choudhary
- Anuradha Anil Ambedkar

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Appendices

‘A’ PARAM Siddhi-AI Work Reports

Title of the work carried out: 15 classes, including vehicles (car, bus, truck, trailer, bicycle, Motorcycle etc.) and other objects (like pedestrians, animals etc.) Detector for Indian roads.

Name & Designation of the Chief Investigator: Amit Raj, Joint Director

E-mail Id: ramit@cdac.in

Institution Name: Centre for Development of Advanced Computing (C-DAC)

Application Domain:

Image Processing and Computer Vision (IPCV)

Research Challenge/s:

For projects involving surveillance applications, there is a requirement of a detector for vehicles and other objects of interest on roads. Vehicles on Indian roads are numerous and traffic can at best be described as chaotic in a number of places. The existing detectors which work good in lite traffic conditions fail when applied as such in Indian conditions. Also the shape of vehicles vary to a large extent owing to custom modifications and color scheme on trucks etc. Therefore a model trained on Indian datasets is required for Indian conditions.

The International Institute of Information Technology (IIIT), Hyderabad in collaboration with Intel has prepared datasets of objects on roads in Hyderabad and Bangalore cities and their outskirts. The datasets have annotations having unique labels like billboard, auto-rickshaw, animal etc. The full datasets has as many as 46,588 images. The histogram of the pixel distribution of the datasets is as shown below.

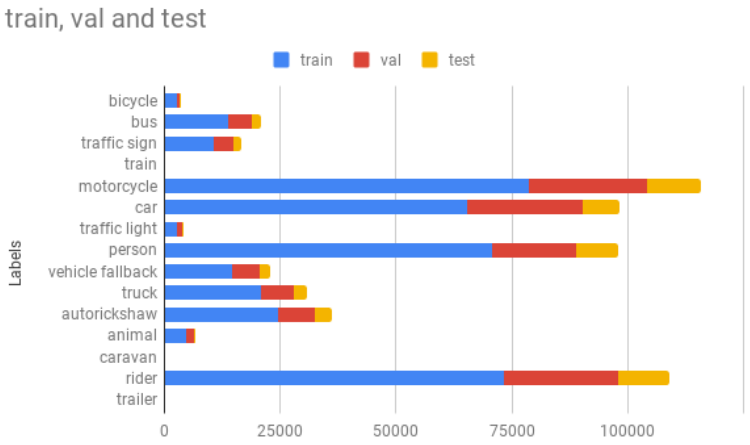


Image Source: https://idd.insaan.iiit.ac.in/dataset/details/

Along with these datasets, the COCO (Common Objects in Context) is a large-scale object detection, segmentation, and captioning dataset. Coco is an extensive collection of annotated images with 80 object categories. The images of relevant classes are carefully extracted from the coco datasets, and a combined data set of 116267 training and 48875 validation images is obtained along with their annotations in the required format.

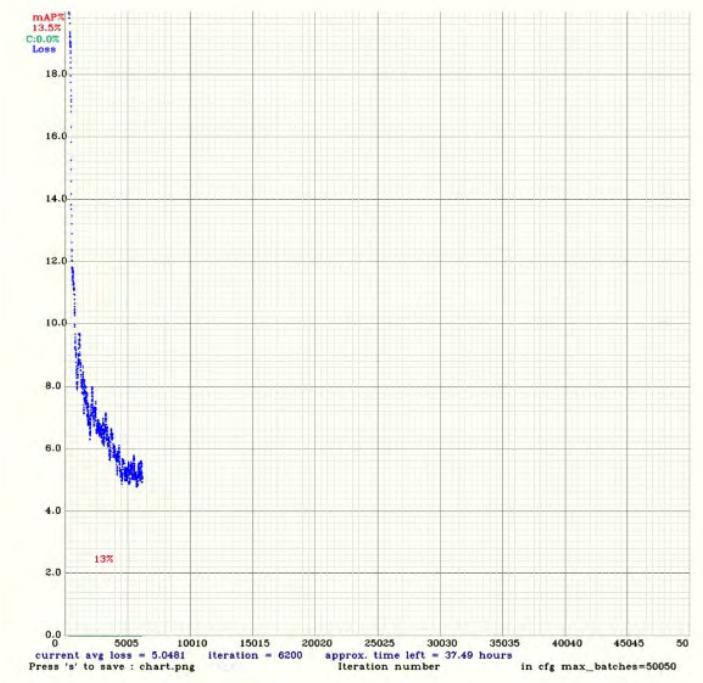
YoloV4 and darknet are used to train the real time, high quality and convincing object detector. The YOLOv4's architecture is composed of CSPDarknet53 as a backbone, spatial pyramid pooling additional module, PANet path-aggregation neck and YOLOv3 head.

Work carried, Milestone, Achievements & Graphs, Plots:

Training of detector with a combined dataset of more than 1 lakh images requires more than 15 days to train on PARAM-Shavak. This training time is cut substantially on Param-Siddhi.

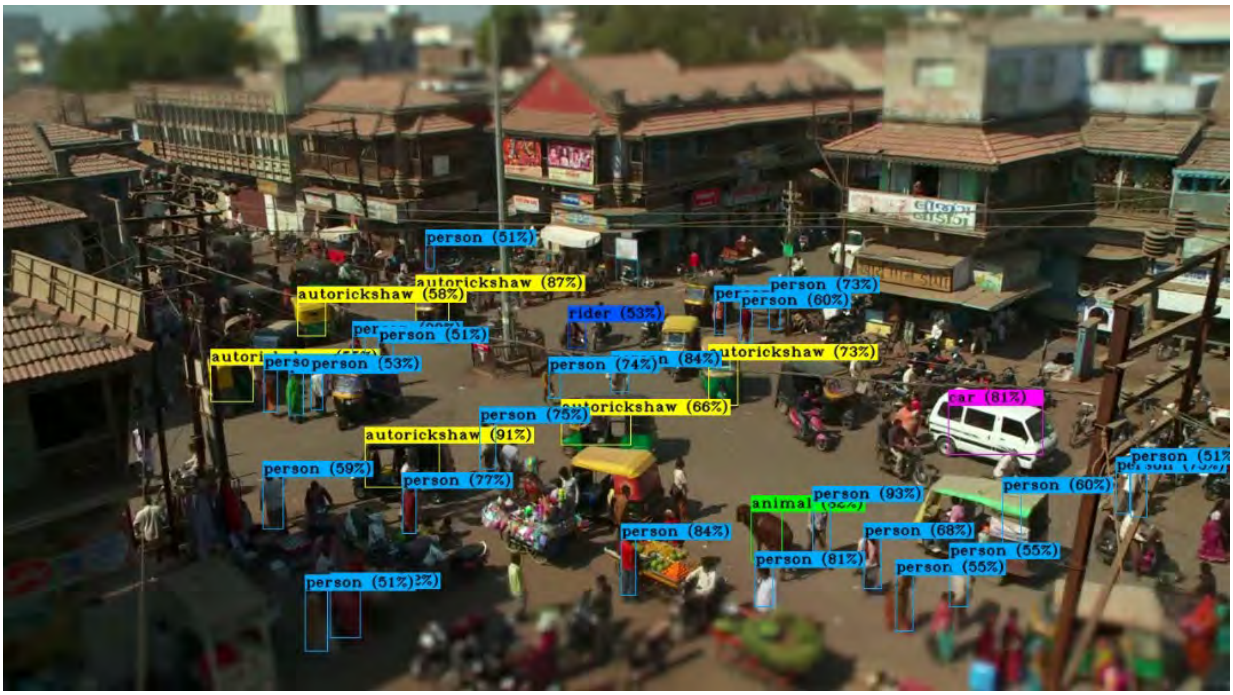
Hyperparameters used for training the detector are as given below:
batch size: 192 with subdivisions 128
learning_rate: 0.001
image width, height = 608
Iterations: 50050

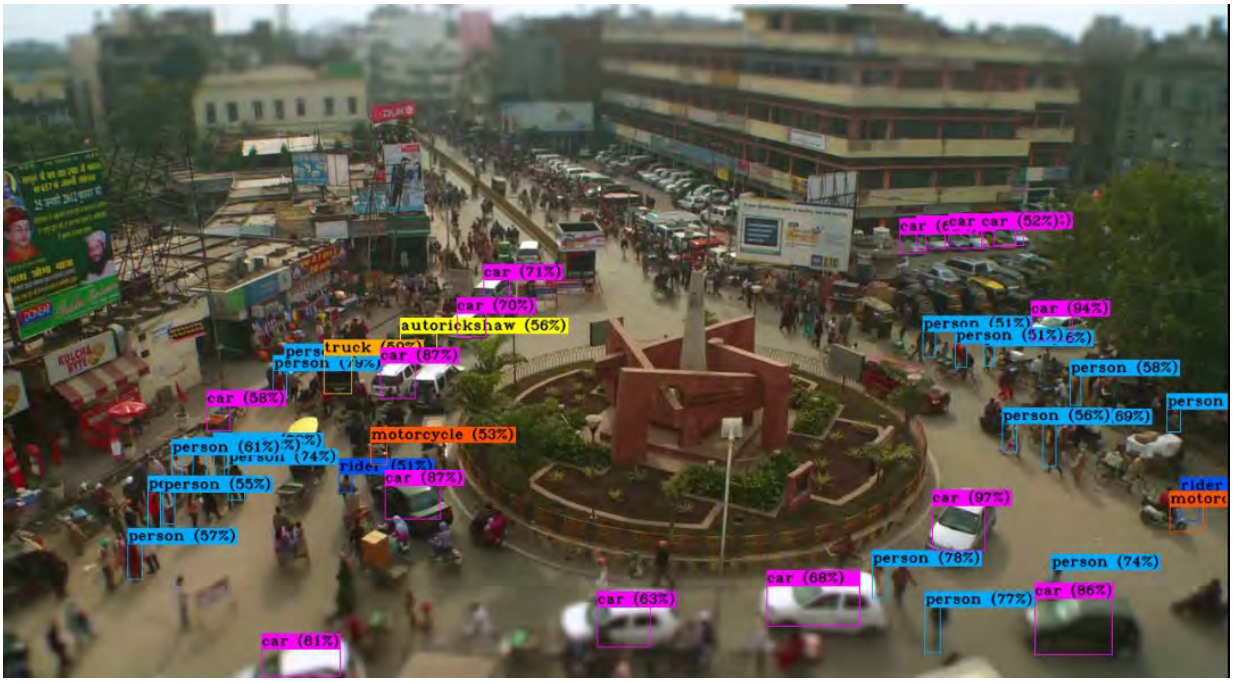
Evaluating the models to find the best is also an intensive job. Models are saved every 10000 steps. The inference is done on all the stored models to finalize the best model with optimum hyper-parameters tuning. Inference also required GPU infra of lesser capacity.



Screenshots from the output video – vehicles and objects of interest detected on roads


train (52%)
car (70%)
car (54%)
car (59%)
motorcycle (57%)
autorickshaw (85%)
autorickshaw (81%)
car (94%)
car (84%)
car (93%)
person (74%)
car (97%)
car (71%)
car (82%)
car (79%)
person (88%)
car (96%)
car (95%)
bus (56%)
car (91%)
car (83%)
car (81%)
car (88%)
autorickshaw (91%)
car (85%)
rider (67%)


person (51%)
autorickshaw (87%)
autorickshaw (58%)
person (73%)
person (60%)
rider (53%)
person (51%)
person (53%)
person (74%)
autorickshaw (73%)
car (81%)
person (75%)
autorickshaw (66%)
autorickshaw (91%)
person (59%)
person (77%)
person (93%)
person (60%)
person (84%)
person (68%)
person (55%)
person (81%)
person (55%)
person (51%)



Video source: https://www.youtube.com/watch?v=KnPiP9PkLAs&t=29s&ab_channel=konzeptunddialog *(www.facebook.com/munichinindia)*

Title of the work carried out: Porting and Scaling of FFTK and TARANG to Param Siddhi

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

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

Institution Name: IIT Kanpur

Application Domain:

Computational Physics, Computational Fluid Dynamics

Research Challenge/s:

In our spectral solver TARANG, based on FFTK, can simulate flows of different types: hydrodynamics, magnetohydrodynamics, thermal convection, rotating flows, etc. In such simulations, FFT operations take around 70% of the total time because of the Alltoall communication operation. So, considering the tremendous power of GPUs, it is imperative to port FFTK to such platform. It seems the fast NVLink and NVSwitch may ease the communication bottleneck.

Work carried, Milestone, Achievements & Graphs, Plots:

We have performed complex to complex FFT & IFFT runs using the multi-GPU functionality [cufftXtSetGPUs] provided by the cufftxt. We have completed these test runs for both single and double precision C2C FFT & IFFT. Besides, we have also checked the timings with a single ROM processor for comparison. In Fig. 1, we have summarized our findings. Note that we have shown speedups compared to a single ROM processor with the same workload. Also, we measured the timings for a single pair of forward and backward transforms. As shown in Fig.1, a significant amount of speed-up can be achieved for higher grid resolution. Besides, we need R2C FFT & C2R IFFT for our spectral solver, which we are also trying to run with cufftxt. In addition, we are exploring cufft with python using cupy. We have succeeded in running multi-GPU FFT in python, but optimization is yet to be done.

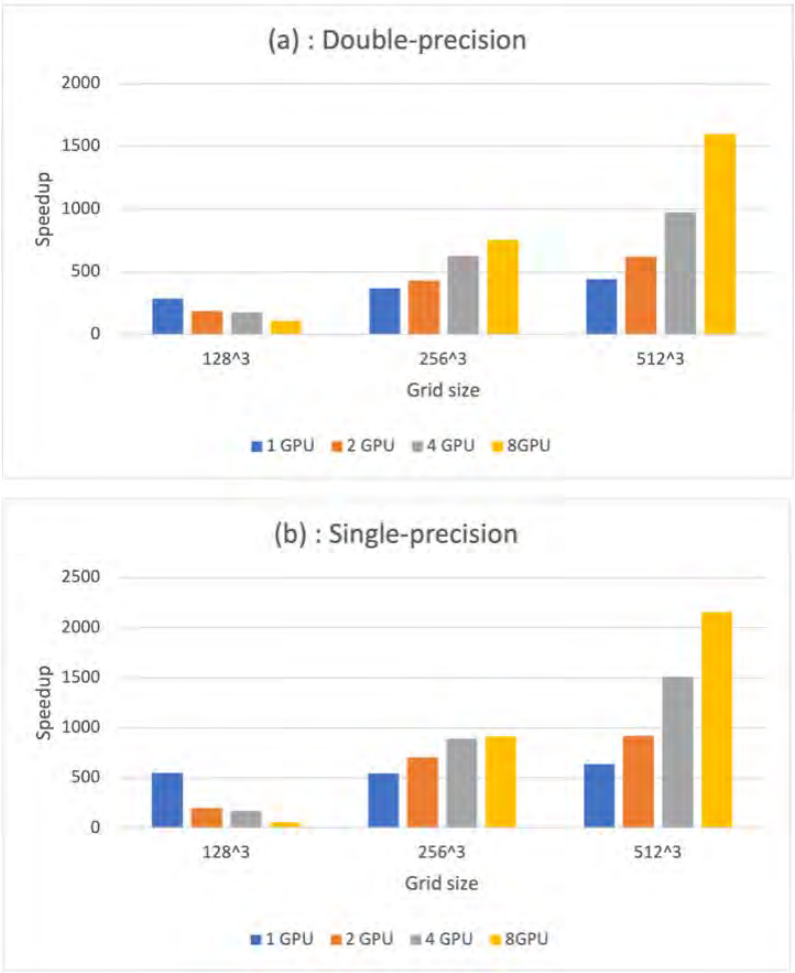


Fig 1: Speedups in performing a single pair of forward and backward Fourier transform in double and single precision with multiple number of GPUs. Note that speedups are with respect to a single ROM processor for the same workload.

Title of the work carried out: Optical character recognition (OCR) for Indian Languages

Name & Designation of the Chief Investigator: Ronak Shah (Joint Director)

E-mail Id: ronaks@cdac.in

Institution Name: Centre for Development of Advanced Computing (C-DAC)

Application Domain:

Image Processing and Computer Vision (IPCV)

Research Challenge/s:

In case of OCR, how characters seen is very important. In case of English, characters are not joined with each other and even order is not changed due to Matra. But same is not true for Indian languages. Indian language is syllabic in nature. One or more chars combined together to make syllable which then decide characters look and order. Number of classes are more in Indian languages as compared to English.

Examples:

hello -> h e l l o

किताब -> क ि त ा ब (Actual order) -> कि ता ब (Visible in image)

Deep learning algorithms are matured enough for solving problems like OCR. Research papers provide hyper-parameters for smaller data-sets which cannot be used as it is for the production environment. All the real world complexities are not considered in the research paper due to the generalization of problem. Real world problems require customization of algorithm and hyper-parameters.

OCR accuracy is depend upon image quality. In real world problems image quality is not as per research papers. so same hyper-parameters cannot used as it is. Images are of low resolution, blur, skewed, text in different colors, with different background, etc.
Training OCR model that can work for Indian language as well as with real world complexities, we need to find optimum hyper parameters. Hyper parameters tuning requires grid search in all the possible values for all the parameters. It is very compute intensive task. We have below mentioned hyper parameters in our system.

batch size : 32 to 128 based on GPU RAM (step size of 8)
learning_rate : 0.1 to 0.0001
Word to vec size : 500 to 2000 (step size of 500)
RNN Layers : 1 to 5 (step size of 1)
RNN size (Units) : 500 to 2000 (step size of 500)

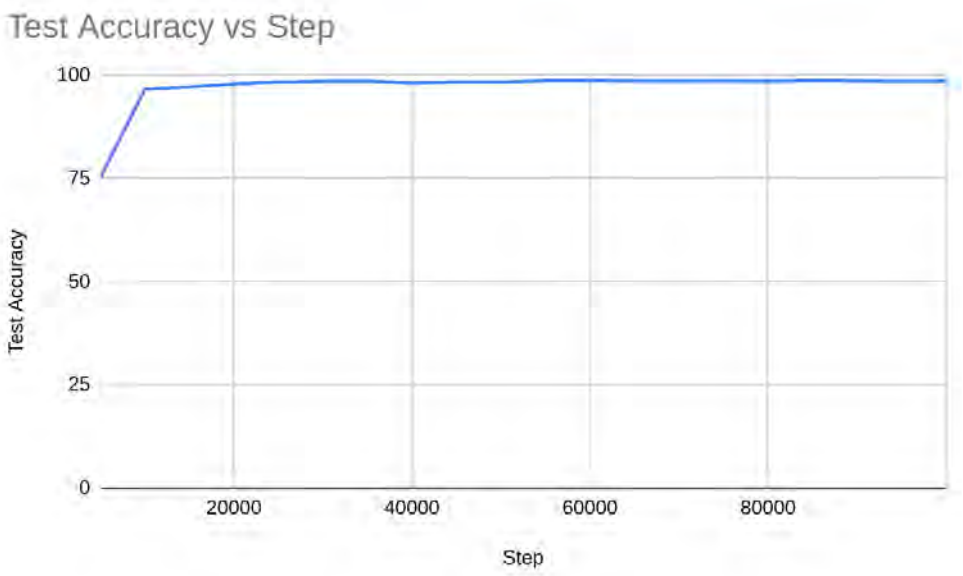
Training of single combination required 12 hours of time on PARAM-Shavak. To run every combinations requires huge GPU infrastructure.

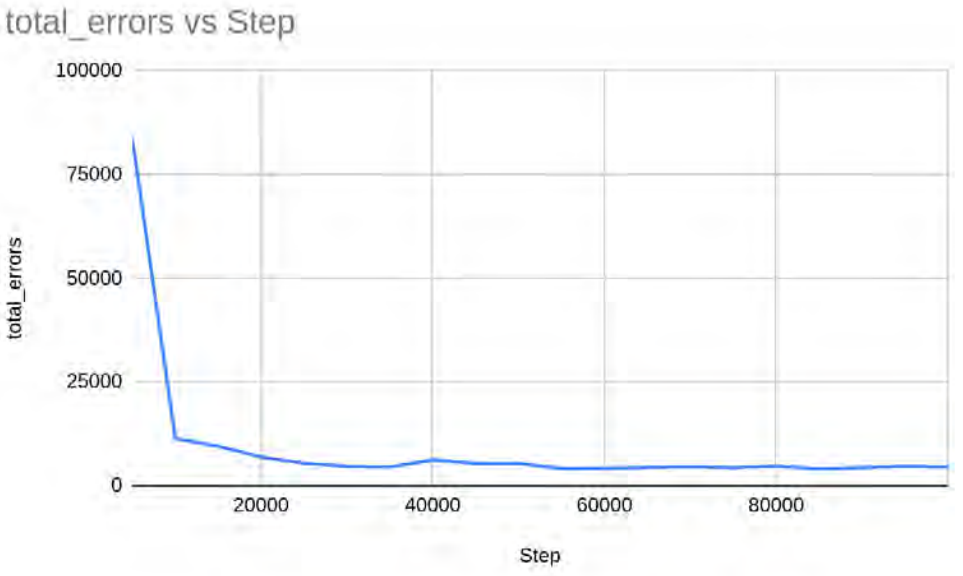
Another challenge is to find best model among all the above trained models. Models are saved after each 5000 steps of 100000 steps. It means 20 models are stored for single hyper parameters setting. Inferencing must be done on all the stored models across all the combinations and finalize best model with optimum hyper-parameters tuning. Inferencing also required GPU infra but of less capacity.

Work carried , Milestone, Achievements & Graphs, Plots:

I have trained OCR engine using Encoder-Decoder architecture and PyTorch deep learning framework. Total training images are 116565. Total number of parameters in network are 13,981,600 (Approx 13 Million parameters). Accuracy is calculated using Levenshtein distance at character level.

Achieved highest accuracy of 98.55% on test data at 85000 steps.





Title of the work carried out: Transitions in flow past a circular cylinder

Name & Designation of the Chief Investigator: Professor Sanjay Mittal

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

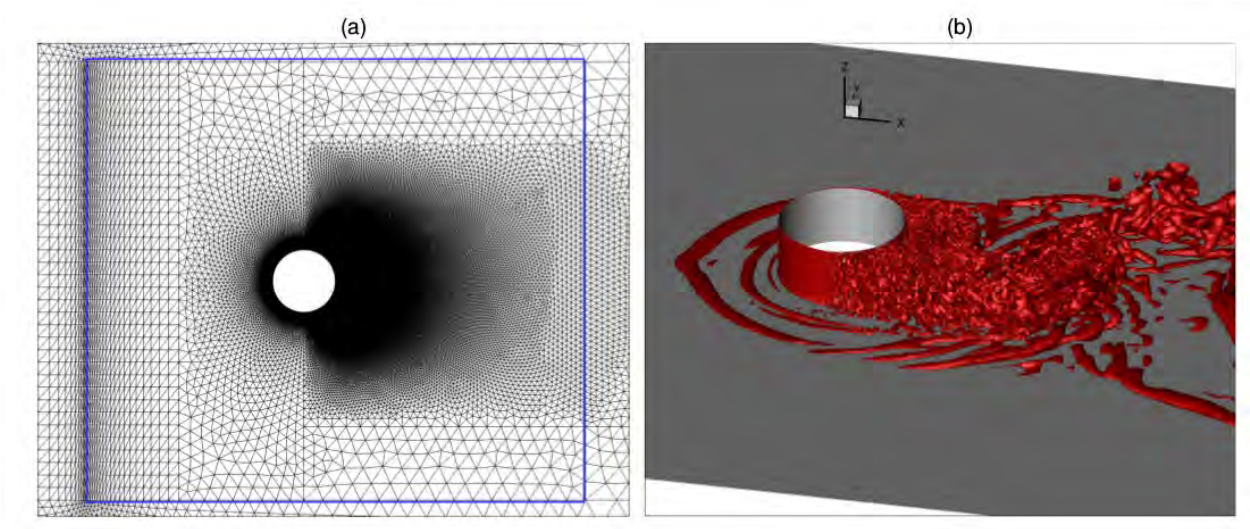
Institution Name: Indian Institute of Technology Kanpur

Research Challenge/s:

The project focuses on understanding the transition of boundary layer in flow past a circular cylinder. This is a challenging problem. This problem involves high numerical accuracy which is obtained by using a very high resolution grid. The PARAM supercomputer computer gives us capabilities to carry out these computations.

Work carried , Milestone, Achievements & Graphs, Plots:

A two-dimensional section of the mesh in the x−y plane is shown in figure 1 (a). The extent of the end plate is shown as well via a black line. The mesh near the leading edge of the end plate as well as upstream of the cylinder, where horse shoe vortices are expected, is suitably modified. To adequately resolve the boundary layer on the end plates, the grid spacing along the span is small and it gradually increases towards the midspan. The grid spacing is 5 × 10−3 D near the end wall and 0.02D at midspan. The circumferential and radial distribution of grid points close to the cylinder is similar to that described earlier. Figure 1 (b) shows the horse shoe vortices in the flow in the presence of a no-slip end plate for Re = 0.4 × 105.



Flow past a circular cylinder (AR = 1) with no-slip condition on the end plates at the lateral boundaries: (a) close-up view of the finite element mesh in the x − y plane. The boundary of the end plate is marked using a black line. b) Q = 1 iso-surface of the instantaneous flow showing the horse shoe vortices in the flow. Only half of the span is shown.

Title of the work carried out:

A. Learning with massive noisy face dataset for obtaining and training a clean dataset for Face Recognition.
   - Learning to automate the cleaning of noisy faces,
   - Auto Generation of face images with Synthetic occlusions,
   - Masked Face Recognition.

B. Indexing Billion of face features (for similarity) on GPU.

Name & Designation of the Chief Investigator: Kapil Mehrotra, Joint Director
Team Members: Karan Khajuria (Project Engineer), Vivek Chandra (Project Engineer)

E-mail Id: kapilm@cdac.in

Institution Name: CDAC Pune

Research Challenge/s:

Massive label noise: Face recognition methods assume that training data are clean. However not true especially when the dataset is in large scale. Also, there is too much difficulty in obtaining a clean dataset for large scale (approx 1M+ subjects) faces recognition. It will require various manual annotators, which can be expensive. The idea here is to learn to annotate from massive noisy label (open and closed) data.

Synthetic Augmentation: In standard face databases, the variations in subject images with respect to occlusions like masks, beard, goggles, specs etc are close to zero. In current scenario, when wearing masks is a necessity. The old face recognition systems are not at all usable. So, we challenged ourselves to synthetically add occlusions like masks, goggles, specs etc on the original face image for generating augmentations. This is an automated process, no human intervention is required.

Limiting the memory usage: This is a key criterion for problems involving large amounts of data. Such as large-scale face recognition in national databases; where millions to billions of face features need to be indexed.

Turnaround time: Here, we are processing millions of face images. For single GPU, the training took around weeks' time. And, then you tune your hyper parameter and go again. This is a sort of a repetitive process till you got the performance sorted, which took months. On a single node of PARAM Siddhi-AI System with 8 A100 GPU's, the train time reduced to hours, which in turn drastically reduced the overall timings.

Work carried , Milestone, Achievements & Graphs, Plots:

A. Learning with massive noisy face dataset for obtaining a clean dataset for Face Recognition: Learning to automate the cleaning of noisy faces

The idea of introducing subclasses for each identity in the label set relaxes intra-class compactness but automates the job of cleaning the data which would have taken a lot of human-effort. This enforces subclasses [5] by nearest intra class center selection and then only keeps the dominant sub-center to achieve intra-class compactness. Thus, results robust and effective facial latent representations.

Experiments:

- **Data-set**: 1M*+ subjects with 7M*+ face images (with open1 and closed2 label noise).
- **Augmented Noise** : 45% - 50%,
- **Architecture**: ResNet-100[1]
- **FLOPS/Parameters**: 24.18 GFLOPS/65.5M
- **Math mode:** Single-Precision Performance (TF32)
- **Distributed GPU Multiprocessing Training**: We set the batch size as 1024 and train models on 8 NVIDIA A100 (40 GB) GPUs s shown in Table 1. For the training of the proposed intra class center, the first round of model with K=5 and K=1 was trained. Then, we drop non-dominant sub-centers (K= 5↓K=1) and high-confident noisy data (>500) by using the first round model. Also, ignored subjects with less than 10 face images.

Training Speed Benchmark	**A100**
Device (Distributed GPU computing)	8 * A100-PCIE-40 GB
Memory VRAM Usage (per)	~ 39 GB
Batch Size	8x128 = 1024
Samples/s	1540 samples/sec

Table 1 Training Speed Benchmark

- **Observations:** For publicly available standard datasets[2][4], Figure 1show the performance of when intra class center K=5 and K=1 for our in-house model:

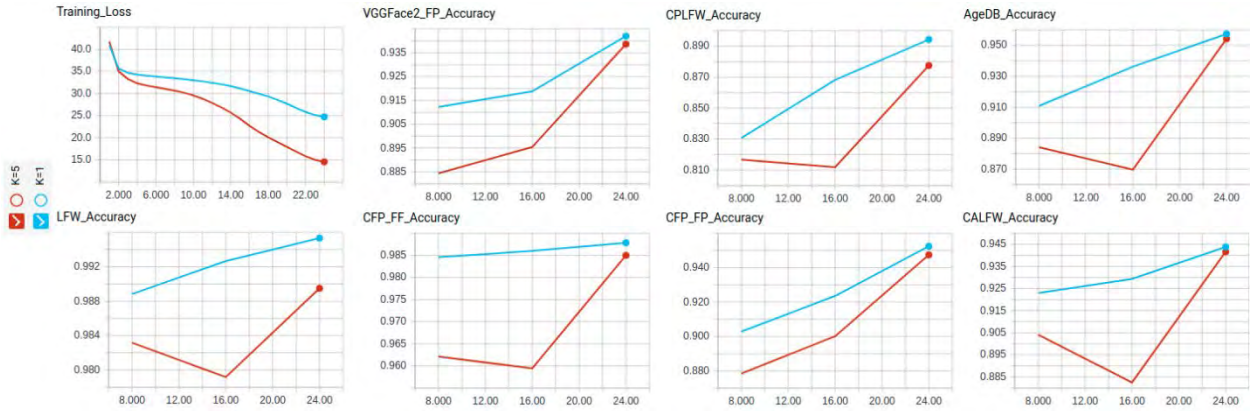


Figure 1 Intra-class performance for K=1 and K=5 on standard datasets.

Angle Selection: By nearest sub-center selection and then only keeps the dominant sub-center to achieve intra-class compactness.

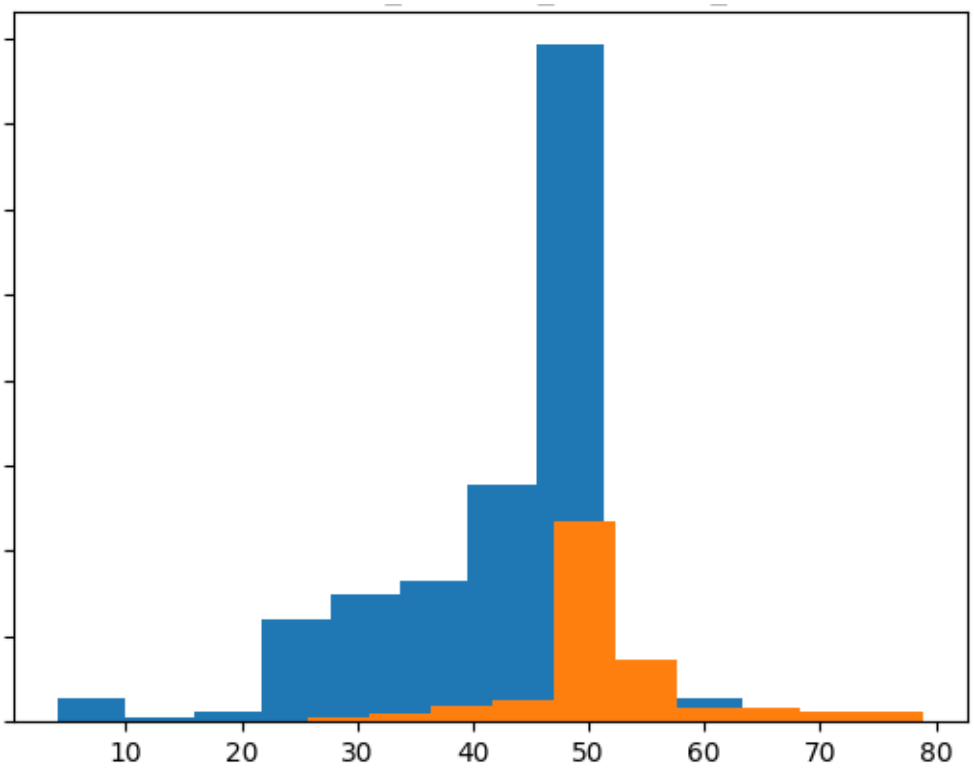


Figure 2 Angles of Dominant samples with their intra-class centres

In Figure 2, blue are dominant samples, orange are non-dominant samples. We, then using the angle threshold ~50, disregarded the samples greater than ~50. The result is the cleaned data-set with ~85K subjects with ~4.8M face images.

i. Auto Generation of face images with Synthetic occlusions & augmentations.

This is the methodology to artificially enrich training data for face recognition under today's circumstances. Used techniques are label preserving transformation usually applied to training images. Such methods improve the accuracy of the system and prevent over fitting. Some of the augmentations used were:

- Scale: Upscale and Downscale image to capture far appearances,
- Compression: Decrease Jpeg and WebP compression of an image,
- Blur: Blur input images using random sized kernels,
- Multiplicative Noise: Multiply image to a random number or array of numbers,
- Color Shifting: Randomly shift values of each channel for a given image. (RGB)
- Occlusions: Leveraging deep learning models, we extract the landmarks from the face images. Using these landmarks, the synthetic occlusions like mask, beards, moustache, specs, goggles was added augmented on the face image.

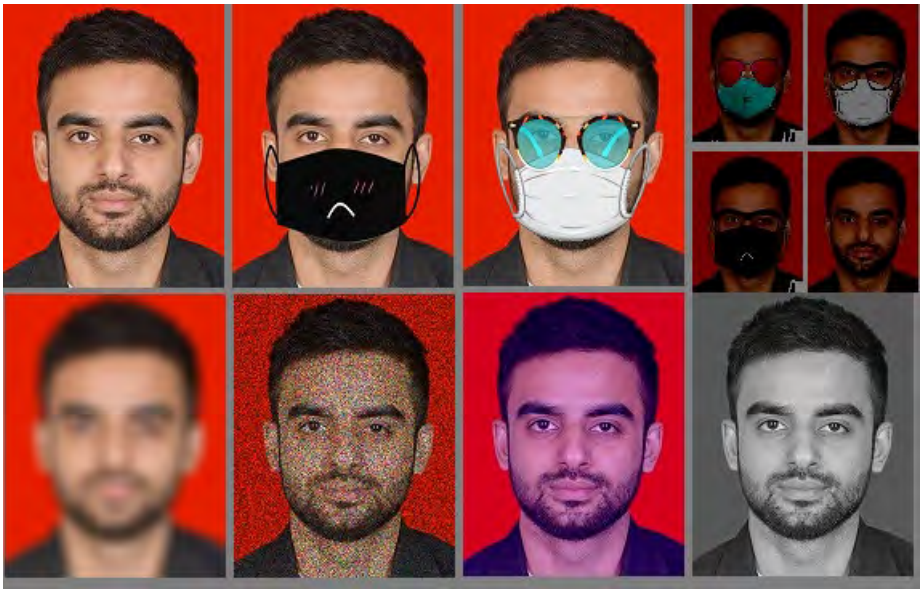


Figure 3 Few snapshots of synthetic augmentations

The synthetic augmentations are automatically generated from the original image. Few of them are shown in Figure 3. Not only singular augmentations, but multiple of them was applied one after the other (as in pipeline) for more robust results. As shown in top right of Figure 3, occlusions like goggles, masks was added onto the original image and then the image is down sampled 4x times with more degradation.

ii. Masked Face Recognition

Stated methodology from i was then used to add variation in data-set by introducing occlusions on sample face images for a robust masked face recognition system can be developed.

Experiments:

- **Data-set**: ~85K^{+} subjects with ~5.8 M face images
- **Architecture**: ResNet-50 | ResNet-100 & Margin Loss [3]
- **FLOPS/Parameters**: 12.61 GFLOPS/43.8M | 24.18 GFLOPS/65.5M
- **Math mode:** Single-Precision Performance (TF32)
- **Distributed GPU Multiprocessing Training**: For both the architecture's, batch size of 2048 was selected. Using Margin loss, the network was trained over 24 epochs as shown in Table 2.

Training Speed Benchmark	**ResNet 50**	**ResNet 100**
Device (Distributed GPU computing)	8 * A100-PCIE-40 GB	8 * A100-PCIE-40 GB
Memory VRAM Usage (per)	~ 32 GB	~ 39 GB
Batch Size	8x256 = 2048	8x256 = 2048
Samples/s	4410 samples/sec	2048 samples/sec

Table 2 Training speed benchmark of Resnet100 vs. Resnet50

- **Observations**: For publicly available standard datasets, Table 3 and Figure 4 shows the performance of our in-house model:

Standard Validation Datasets	ResNet100	ResNet50
VGG2 Frontal Profile	95.26%	95.44%
AgeDB	97.98%	97.95%
CALFW (Cross-Age LFW)	96.20%	95.89%
CFP_FF (Celebrities in Frontal Profile in the Wild : frontal to frontal verification)	99.8%	99.78%
CFP_FP (Celebrities in Frontal Profile in the Wild : frontal to profile verification):	98.42%	98.14%
CPLFW (Cross-Pose LFW)	93.13%	92.58%
LFW (Labelled faced in the Wild)	99.74%	99.78%

Table 3 Performance of ResNet100 vs. ResNet50 on Val set

Figure 4 Performance of Resnet100 vs. ResNet50 on Train & Val dataset

A. Indexing billion of face features

The idea is to decompose the space of Face features into Cartesian products of low dimensional subspaces and quantize each subspace separately. The Euclidean distance is used for the similarity search in embedding space. Quantization is a destructive process which has been extensively studied in various theories. The memory cost of storing the index is far less than storing floating points of high dimensional vectors.

Indexing billions (100 crore) of facial features (on GPU device) [6] in limited amount resources. The product quantization (PQ) is used for resource consumption.

- **Data-set**: 100 crore+ (1B[!]) augmented facial features.
- **Technique**: Similarity search methods that achieve near-optimal performance on GPUs.

- **Distributed GPU Multiprocessing Training**: The indexing of 100 crore features with 128 dimensions (100 crore x 128) was done 2 xA100-PCIE-40GB.
    - The timing of indexing done on GPU for 100 crore was reduced to just 2419.87 secs from 3.5 days on CPU as shown in Table 4 and Table 5.
    - We utilized 2 cards for this, each with 40 GB VRAM. The GPU memory consumption (VRAM) was around 28 GB per card so a total of 56 GB.
    - The index file size is around 38 GB (same as in case of CPU).

CPU (56 cores) (96 GB RAM)	# Data	# Centroids	# PQ	# Training data points	Total Time for Training	Data Add statistics		File write (in secs)
						# Addition in single iteration	Total time for adding (in secs)	
	100,00,41,199	32768	32	1304515	**3943.01**	260903	**306640 (3.5 days)**	34.96

Table 4 Indexing on CPU

# GPU (A100)	# Data	# Centroids	# PQ	# Training data points	Index Training time (in seconds)				Data Add statistics				File write (in secs)
					CPU to GPU time (in secs)	Training time (in secs)	GPU to CPU time (in secs)	Total Time for Training	# Addition in single iteration	Total Add time (in secs)	GPU to CPU time (in secs)	Total time for adding (in secs)	
2	100,00,41,199	32768	32	1304515	1.27	16.26	0.1	**17.63**	260903	2379.38	40.49	**2419.87**	34.96

Table 5 Indexing on GPU

References

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[6] J. JOHNSON, M. DOUZE AND H. JÉGOU, "BILLION-SCALE SIMILARITY SEARCH WITH GPUS," IN IEEE TRANSACTIONS ON BIG DATA, DOI: 10.1109/TBDATA.2019.2921572.

Title of the work carried out: Exploration of LINUX tools and HPC using CUDA

Name & Designation of the Chief Investigator: Dr. Manish Modani & Principal Solution Architect

E-mail Id: ganinampelly979@gmail.com

Institution Name: NVIDIA

Application Domain:

CFD, HPC

Research Challenge/s:

We faced Issues from the PARAM Siddhi system, like
MPI isn't installed on all the nodes
GPU0 on node 1 was not behaving properly for some days
Simple MPI code isn't running on multinode.

Work carried , Milestone, Achievements & Graphs, Plots:

I was learning the basics of Linux system related stuff, writing sample cuda codes and learning the debugging tools along with profiling the codes using Nsight Systems. Recently, we finished installing SPECFEM3D code to perform multinode, multi GPU performance analysis.

Title of the work carried out: Numerical Investigation of Flow inside a 3D Supersonic Y Duct

Name & Designation of the Chief Investigator: Thesis Supervisor – Dr. Sanjay Mittal, Professor

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

Institution Name: IIT Kanpur

Application Domain:

Air Intakes are crucial part of most modern passenger and military aircrafts. The work aims to simulate the flow phenomena inside the duct at various side slip angles and different back pressure ratios.

Research Challenge/s:

Faced difficulty in preparing the appropriate mesh for sufficient resolution of various flow phenomena. Implementation of the back pressure and side slip angle to the flow.

Work carried , Milestone, Achievements & Graphs, Plots:

Successfully implemented the back pressure to both symmetric and asymmetric flow.
Successfully Developed the flow for higher back pressure cases with sufficient resolution of various flow phenomena like shock boundary layer interaction.

Title of the work carried out: FLAME Solver – Scalable Asynchrony-Tolerant Solver for Compressible Navier-Stokes Equations

Name & Designation of the Chief Investigator: Dr. Konduri Aditya, Assistant Professor

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

Institution Name: IISc (Indian Institute of Science, Bangalore)

Application Domain:

Computational Fluid Dynamics

Research Challenge/s:

Ensuring accuracy with asynchronous strategy for inter GPU communication. Scalable method for exascale

Work carried, Milestone, Achievements & Graphs, Plots:

We have started using Param Siddhi from March 1, 2021. Most of the work until now has been code development on other machines. We have matched accuracy with some existing code and have just started profiling on the A100 GPUs on Param Siddhi.

Title of the work carried out: Automatic Speech Recognition

Name & Designation of the Chief Investigator: S. Umesh, Professor, IIT Madras

E-mail Id: umeshs@ee.iitm.ac.in

Institution Name: Indian Institute of Technology Madras

Application Domain:

Automatic Speech Recognition

Work carried, Milestone, Achievements & Graphs, Plots:

Installation of softwares like ESPNET, KALDI, FAIRSEQ etc. Basic ASR experiments for verifying baselines.

Title of the work carried out: Scalable finite-element based real-space algorithms for quantum mechanical modeling of materials at extreme-scale.

Name & Designation of the Chief Investigator: Dr. Phani Motamarri – Assistant Professor, Department of Computational and Data Sciences, Indian Institute of Science (IISc) Bangalore.

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

Institution Name: Indian Institute of Science (IISc) Bangalore

Application Domain:

Computational Materials Science

Research Challenge/s:

Development of novel algorithmic approaches and implementation advances for fast, scalable and accurate quantum mechanical calculations using density functional theory.

Work carried, Milestone, Achievements & Graphs, Plots:

Access to PARAM Siddhi is obtained a month ago on Feb 25, 2021. Primary goal in the current work is to demonstrate extreme-scale readiness of in-house developed computational methods and algorithms to conduct large-scale quantum mechanical calculations using density functional theory (DFT) for material modeling applications employing real-space based finite-element discretization. To this end we are currently working on developing finite-element based computational methods for solving large-scale generalized eigenvalue problem resulting from using state-of-the-art projector-augmented-wave (PAW) potentials for DFT calculations in conjunction with semi-local exchange-correlation functionals (SCAN). Furthermore, novel algorithmic approaches focusing on reduced data access costs in accomplishing finite-element discretized matrix-vector multiplication are also being developed. Finally, the proposed extreme- scale computational capabilities will be leveraged to gain a fundamental understanding of the mechanisms that cause dendritic growth in Li-La-Zr-O (LLZO) solid electrolyte in the presence of electric-field.

Title of the work carried out: Application performance and analysis at Scale. The applications include WRF, GROMACS, SPECFEM3d etc. These applications performances, first time, analyzed on multi-node, multi-GPUs on PARAM SIDDHI AI system.

Name & Designation of the Chief Investigator: Dr. Manish Modani, Principal Solution Architect

E-mail Id: mmodani@nvidia.com

Institution Name: NVIDIA

Application Domain:

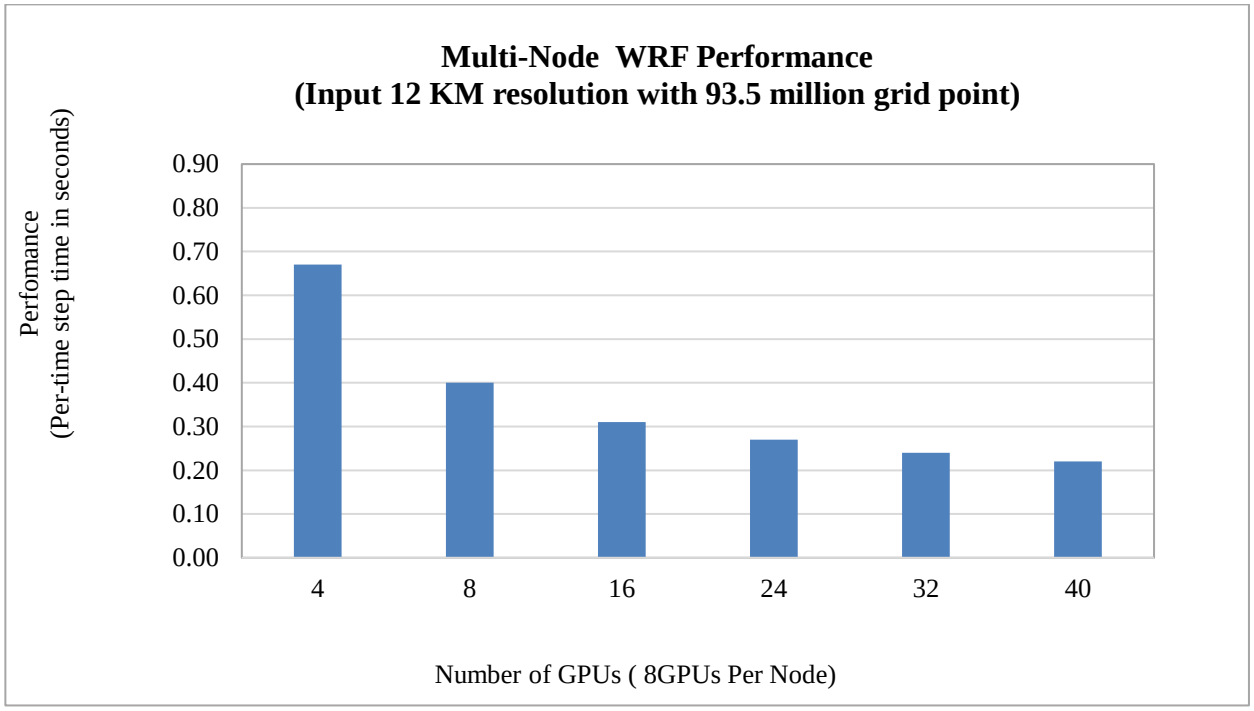
Weather, Molecular Dynamics, etc

Research Challenge/s:

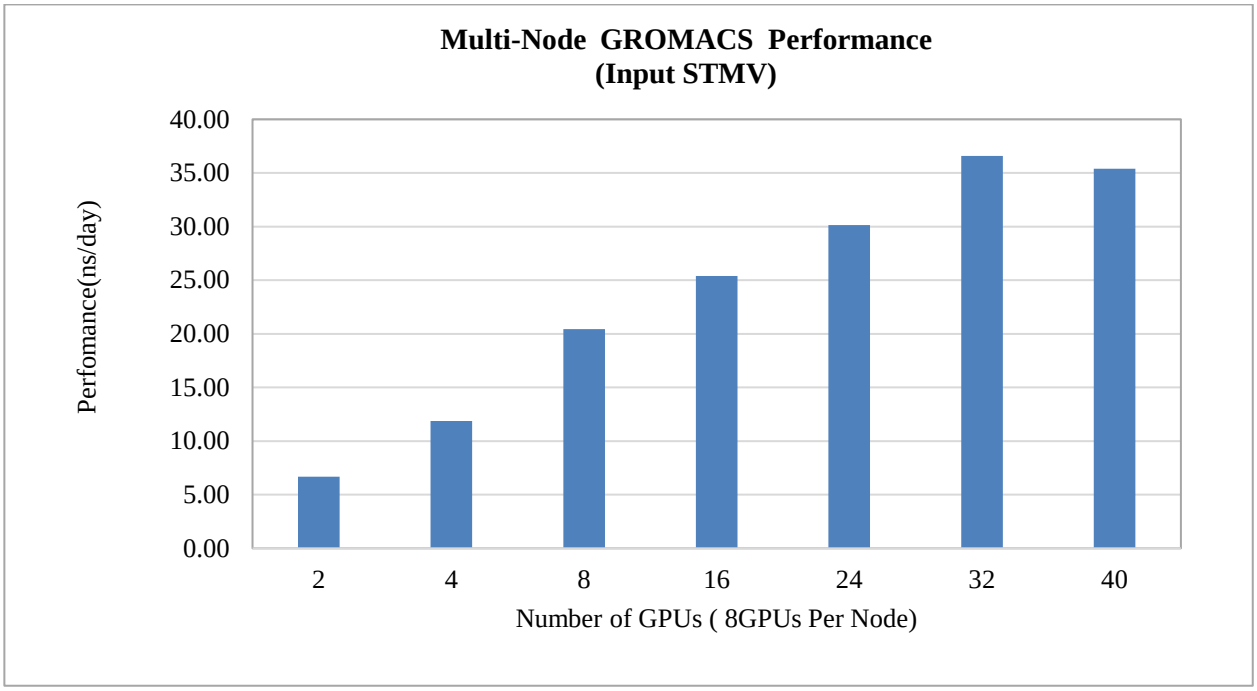
First time, applications performance analyzed on 5 nodes (upto 40 A100 GPUs)

Work carried, Milestone, Achievements & Graphs, Plots:

(a) WRF Scalability:



(b) GROMACS Scalability


Multi-Node GROMACS Performance
(Input STMV)
Perfomance(ns/day)
40.00
35.00
30.00
25.00
20.00
15.00
10.00
5.00
0.00
2
4
8
16
24
32
40
Number of GPUs (8GPUs Per Node)

Title of the work carried out: Automated Lung Ultrasound Image Analysis

Name & Designation of the Chief Investigator: Dr. Mahesh Raveendranatha Panicker, Assistant Professor, IIT Palakkad

E-mail Id: mahesh@iitpkd.ac.in

Institution Name: Indian Institute of Technology Palakkad

Application Domain:

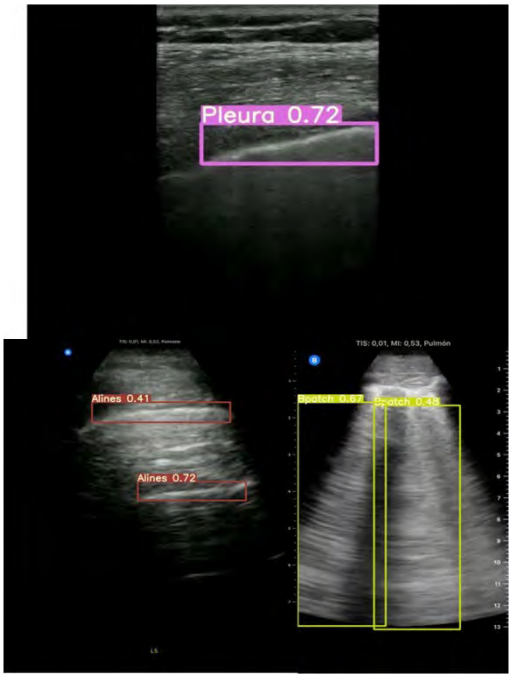
ML/DL for Ultrasound Imaging

Research Challenge/s:

Started using the system from early March and it is just over a month. Initially faced challenges in installing custom libraries, but with NGC it appears to be solved. There are no further issues as such.

Work carried, Milestone, Achievements & Graphs, Plots:

The work has started only from mid of March. The main work involves the automated labelling of various landmarks in lung ultrasound videos/images. Based on the same, the image quality metrics as well as a severity of the lung infection will be predicted for clinical assistance. Some initial results of the automated algorithm are as below.



Title of the work carried out: Design and development of End-to-End Automatic Speech Recognition system for Hindi & Indian English languages using cutting-edge deep learning algorithms, frameworks and pipeline.

Name & Designation of the Chief Investigator: Mahesh Bhargava

E-mail Id: mbhargava@cdac.in

Institution Name: Centre for Development of Advanced Computing (C- DAC)

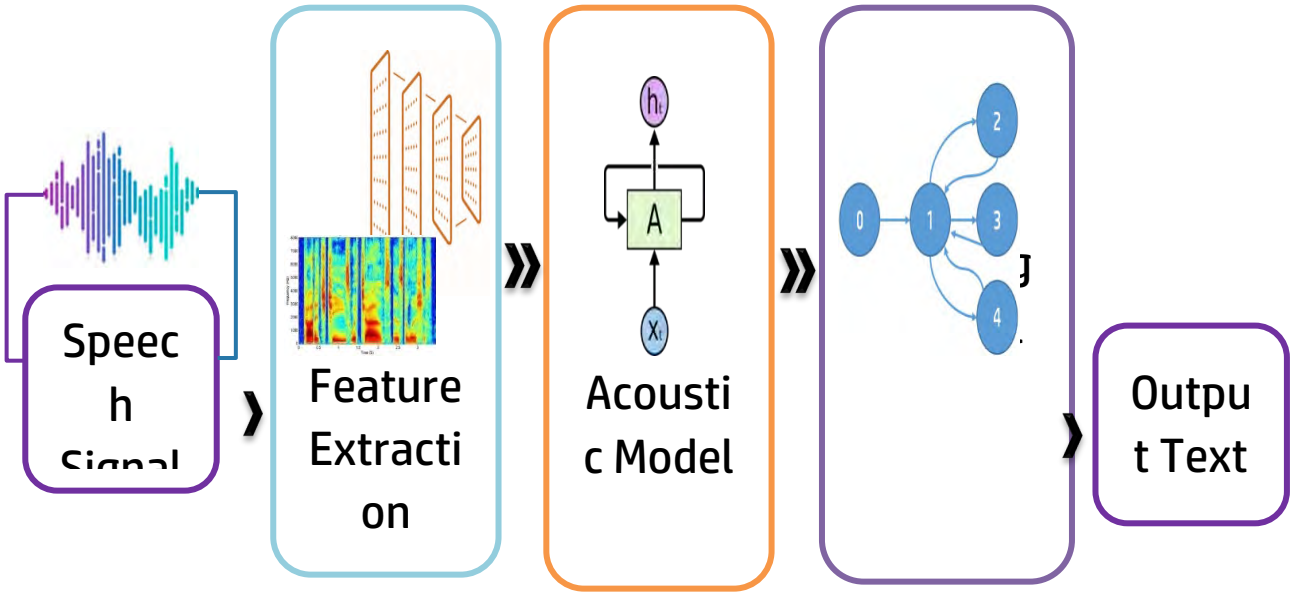
Application Domain:

Automatic Speech Recognition [ASR]

Research Challenge/s:

Design and development of End-to-End Automatic Speech Recognition system for Hindi & Indian English languages using cutting-edge deep learning algorithms, frameworks and pipeline.

ASR is the process of transcribing raw audio signal into stream of text.



ASR Benchmarking on PARAM Siddhi-AI:

Training and Inferencing on PARAM Siddhi AI				
SL#	**Language**	**Speech Corpus (Hrs.)**	**Training Time (Hrs.)**	**Inference Time**
1.	**English**	**2600**	**23:00**	**1Hrs. data in 1Sec.**
2.	**Hindi**	**400**	**04:30**	

System Configuration
Compute Type: DGX A100
No. of GPUs: 8
GPU Memory: 40GB

Tools/Framework used for ASR on PARAM Siddhi-AI :

Tool/Software/Lib	
ASR Speech Toolkit	**Kaldi and GStreamer**
DL Library	**PyTorch**
NVIDIA Framework/Lib	**NeMo, Jarvis, CUDA Toolkit, cuDNN**

Kaldi: It is an open-source speech recognition toolkit, intended for use by speech recognition researchers and professionals.

NeMo: NeMo is an open-source toolkit for developing state-of-the-art conversational AI models.

Jarvis: Jarvis is an application framework for multimodal conversational AI services that delivers real-time performance on GPUs.

Targeted Applications of ASR on PARAM Siddhi-AI

- Conversation Indic-AI Stack
- Speech to Speech Machine Translation
- Automatic subtitle generation
- Dictation application

- Voice command & control
- Personal assistant systems
- Defense & intelligence agencies
- Accessibility
- Video Transcription

'B' Financials

The finance section would cover the overall expenditures towards running the operations of clusters at NPSF. Commercial Invoices were raised for PARAM Yuva II services, and the CPU Time Invoices were raised regarding the utilization of computing resources of the PARAM Yuva II cluster.

Operational expenditure would include the AMCs of Power-Cooling Infra, i.e.,PAC (Precision Air Conditioners), UPS (Uninterrupted Power Supply), DG (Diesel Generators), Synchronization panel Breaker switch, and the charges towards the consumption of electricity and diesel.

In total Year2020 total expenditure comes to around Rs.1.71 crores.

Commercial Invoices are being raised for the users paying the charges towards using the PARAM Yuva II compute resources. In 2020, close to 70k amount of Commercial Invoices had been raised.

Monthly invoices were raised regarding the utilization of compute resources of PARAM Yuva II cluster by user's jobs. These invoices are being sent to the individual Chief Investigator of the Projects during Year2020 (i.e., from January to December). The accumulated value of the CPU time consumed for the Year 2020 is 43047643CPU Hours. E-Money Equivalent of the consumed CPU Time is around Rs. 13,68,97,468.00 (Thirty teen Crores Sixty-eight Lakhs and Ninety-Seven Thousand and Four hundred Sixty-eight only).

Table: Financials

Sr.No.	ITEMS Received	INR
1	Total Commercial Invoices raised for the use for PARAM Yuva II services	70K

Table: Financials

Sr. No.	**Expenditure**	**INR**
1	AMC for PAC	4.0 lac
2	AMC for UPS	4.5 lac
3	AMC DG Set	1.5 lac
4	AMC for Synchronization Panel	30 k
5	AMC for Breaker Switch	55 k
6	Diesel Consumed	10 lac
7	Electricity Consumed	150 lac
	Total	170.85 lac

Note: Figures in INR mentioned above are not to be considered as an exact expenditure. Manpower / Staffing cost is not shown

‘C’ Users across Institutions

Below is the list of NPSF users across Institutions

Table : Users across Academic Institutions

State	Academic Institutions	No. of Users
Assam.	Assam University, Silchar.	1
	Dibrugarh University, Dibrugarh	3
	Indian Institute of Technology (IIT), Guwahati.	22
	National Institute of Technology (NIT), Silchar.	3
Bihar	Central University of South Bihar (CUSB), Patna	1
	Indian Institute of Technology (IIT), Patna.	10
Chandigarh	Panjab University, Chandigarh.	8
Delhi	Guru Gobind Singh Indraprastha University, Delhi	3
	Indian Institute of Technology (IIT), Dehli.	8
	Indraprastha Institute of information technology, Delhi	4
	Jamia Millia Islamia University, New Delhi.	5
	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

State	Academic Institutions	No. of Users
	Government Engineering College, Modasa	1
	Indian Institute of Technology (IIT), Gandhi Nagar	10
	Sardar Vallabhbhai National Institute of Technology (SVNIT) , Surat.	14
	St. Xaviers College, Ahmedabad.	1
Haryana	Central University of Haryana (CUH), Jant-Pali	5
	Kurukshetra University, Kurukshetra	5
Himachal Pradesh	Central University of Himchal Pradesh (CUHIMACHAL), Shahpur	2
	Himachal Pradesh University, Shimla.	7
Jammu and Kashmir	University of Kashmir, Srinagar	2
Jharkhand	Indian Institute of Technology (Indian school of Mines) (IITISM) , 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, Mysuru.	2
Kerala	Indian Institute of Science Education and Research (IISER), Thiruvananthapuram	3
	Indian Institute of Space Science and Technology (IIST), Thiruvananthapuram	2
	Indian Institute of Information Technology (IIIT) Kottayam	3
	National Institute of Technology (NIT), Calicut	1
Madhya Pradesh	ABV - Indian Institute of Information Technology and Management (ABV- IIITM), Gwalior.	6

State	Academic Institutions	No. of Users
	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
	Indian Institute of Science Education and Research (IISER), Pune.	68
	Indian Institute of Technology (IIT),Bombay	263
	JSPM TSSM College, Pune	1
	Maharashtra Institute of Technology, Pune	1
	Padmabhooshan Vasantdada Patil Institute of Technology (PVPIT), Pune	3
	Rashtrasant Tukadoji Maharaj Nagpur University (RTMNU) , Nagpur	2
	Savitribai Phule Pune University, Pune.	43
	Shivaji University, Kolhapur	2
	Swami Ramanand Teerth Marathwada University (SRTMUN), Nanded	2
	Symbiosis Institute of Technology (SIT), Pune	1
	Tetrahydrix Engg. Pvt. Ltd. (TEPL), Pune	1
	Visvesvaraya National Institute of Technology (VNIT), Nagpur.	10
	Whistling Woods International Institute (WWII), Mumbai.	2
Mizoram	Pachhunga University College , Aizawl	1

State	Academic Institutions	No. of Users
Odisha	Indian Institute of Technology (IIT), Bhubaneswar.	6
	Indian Institute of Science Education and Research (IISER),Berhampur	4
	Kalinga Institute of Industrial Technology (kiit), Bhubaneswar	2
	National Institute of Technology Rourkela (nitrkl)	1
Pondicherry	Pondicherry University, Pondicherry.	5
Punjab	Dr. B R Ambedkar National Institute of Technology, Jalandhar	1
	Guru Nanak Dev University, Amritsar.	1
	Indian Institute of Science Education and Research (IISER), Mohali.	2
	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
	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
	Shanmugha Arts, Science, Technology & Research Academy (SASTRA), Thanjavur	3
	University of Madras, Chennai.	1
	SRM Institute of Science and Technology,Kattankulathur	3

State	Academic Institutions	No. of Users
Telangana	BITS Pilani, Hyderabad	2
	CMR College of Engineering & Technology (CMRCET) , Hyderabad	2
	GITAM university , Hyderabad	1
	Indian Institute of Technology (IIT), Hyderabad.	35
	International Institute of Information Technology (IIIT), Hyderabad	4
	Osmania University, Hyderabad.	3
	Professor Jayashankar Telangana State Agricultural University (PJTSAU), Hyderabad.	1
	University of Hyderabad, Hyderabad.	1
Tripura	Women's College, Agartala	1
Uttar Pradesh	Aligarh Muslim University (AMU), Aligarh	7
	Amity University, Noida	2
	Banaras Hindu University, Varanasi.	3
	Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur	1
	Galgotias University, Greater Noida	1
	GLA University, Mathura	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	**814**

State	Research Institutions	No. of Users
Assam	Institute of Advanced Study in Science and Technology (IASST), Guwahati.	4
Delhi	National Informatics Centre, Delhi	2
Gujarat	Indian Space Research Organisation (ISRO),Ahmedabad	5
	Physical Research Laboratory (PRL), Ahmedabad	3
Haryana	Dr.Vijay Kumar Foundation, Gurgaon.	10
	Regional Centre for Biotechnology, Faridabad	2
	Translational Health Science and Technology Institute (THSTI) , Faridabad	4
Karnataka	GARUDA	165
	Indian Air Force (INAF), Bengaluru.	1
	Indo-Korea Science and Technology Centre (IKST),Bengaluru	1
	Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru.	11
	Raman Research Institute (RRI),Bengaluru	3

State	Research Institutions	No. of Users
Madhya Pradesh	UGC DAE Consortium for Scientific Research, Indore	1
Maharashtra	Bhabha Atomic Research Centre (BARC), Mumbai.	1
	Centre for Development of Advanced Computing (CDAC)	157
	CSIR-National Chemical Laboratory (CSIR-NCL), Pune.	8
	E-teacher	2
	Inter-University Centre for Astronomy and Astrophysics (IUCAA), Pune	7
	National Centre for Radio Astrophysics(NCRA), Pune	6
	The Institute of Science, Mumbai	2
	UM-DAE Centre for Excellence in Basic Sciences, Mumbai.	3
Manipur	Institute of Bioresources and Sustainable Development (IBSD),Imphal	2
Odisha	National Institute of Science Education and Research (NISER), Bhubaneswar	2
Punjab	National Agri-Food Biotechnology Institution (NABI),Mohali	1
Tamil Nadu	Central Electro Chemical Research Institute (CSIR),Karaikudi	4
	DRDO-BU Centre for life Sciences, Coimbatore	4
Uttar Pradesh	Bharat Petroleum Corporate Research and Development Centre, Noida.	2
	Harish-Chandra Research Institute(HRI), Allahabad	2
West Bengal	Central Inland Fisheries Research Institute (CIFRI),Kolkata	2
	Indian Association for the Cultivation of Science (IACS), Kolkata.	1
	Saha Institute of Nuclear Physics,Kolkata	2
	S. N. Bose National Center for Basic Sciences, Kolkata	1
	Total	**421**

‘D’ Projects Enrolled during Year 2020

The list of projects from various institutions using NPSF compute time with the details of chief investigator and the number of users are included in this appendix.

Table 1: Projects using NPSF compute time

Institute	Project	Research Field	Chief Investigator	No. of users
Biological and Life Sciences, Ahmedabad University	Drug Design and Molecular Simulation Studies of Beta and Gamma Secretase and Beta Amyloid Proteins and Other Proteins Involved in Neurodegeneration Diseases	Bio Sciences	Dr. Vivek Tanavde	2
Center for Modeling and Simulation,Savitribai Phule Pune University, Pune.	The prime objective of my project is to study the effect of defects on thermal transport and electronic transport of advanced materials using a novel atomistic approach	Material Sciences	Dr. Ankita Katre	1
Central University of Haryana (CUH), Jant-Pali	Mosx integrated porous surfaces for catalytic hydrogen generation via water splitting	Uncategorized	Dr. Prakash Kanoo	2
Central University of South Bihar (CUSB), Patna	Identification of potential natural inhibitors against SARS-Covid19	Uncategorized	Dr. Krishna Kumar Ojha	1
Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur	Molecular dynamics simulation of a nano-sized magnetic molecular system with a nemtogen	Uncategorized	Mr. Manoj Kumar Dwivedi	1
Dr. B R Ambedkar National Institute of Technology, Jalandhar	Many-body correlations effects on the one-dimensional electorn fluid	Uncategorized	Dr. Vinod Ashokan	1
Galgotias University, Greater Noida	Computational modelling of 2D materials for energy storage	Uncategorized	Dr. MD Shahzad Khan	1
H.P.T Arts and R.Y.K. Science College, Nasik	Optimizing the morphological , electric and electrochemical properties of Tio2 Polythiophene and pedot	Material Sciences	Dr. A.B. Chourasia	2
Indian Institute of Engineering Science and Technology, Shibpur	Predictive Design of High-entropy Alloys	Material Sciences	Dr. Gautam Anand	1
Indian Institute of Information Technology (IIIT), Kottayam	Design high performance energy devices.Modeling and simulation ohigh energy density supercapacitors and Li/Na-ion batterie and high efficiency Solar cells will be performed.	Uncategorized	Dr. Boddepalli SanthiBhushan	4
Indian Institute of Science Education and Research (IISER), Pune.	Study of CdS and CdTeS quantum dots decorated on TiO2 nanowires	Material Sciences	Dr. Prasenjit Ghosh	7

Table 1 – Continued from previous page

Institute	Project	Research Field	Chief Investigator	No. of users
Indian Institute of Science Education and Research (IISER), Pune	Selective hydrogenation of acetylene on PdGa intermaetallic compounds(As per New TAS From: Selective hydrogenation of acetylene to ethylene on PdGa surfaces and clusters supported on MgO)	Material Sciences	Dr. Prasenjit Ghosh	6
Indian Institute of Technology (IIT),Ropar	Quantum Dynamics of atom-molecular ion Collision Processes	Chemical Sciences	Dr. T. J. Dhilip Kumar	4
Indian Institute of Technology (IIT), Kanpur.	Energy Harvesting Through Bio-inspired Locomotion	Uncategorized	Dr. Ashoke De	4
Indian Institute of Technology (IIT),Bombay	For studies that involve computationally intensivefluid simulations - atmospheric turbulence predictions, computational aeromechanics and aeroelasticity (multidisciplinary involving both structural and fluid dynamics	Computational Fluid Dynamics	Prof. Abhijit Gogulapati	3
Indian Institute of Technology (Indian school of Mines) (IITISM) , Dhanbad	Mapping lithospheric structure of chhotanagpur plateau from SPL-waveform inversion	Uncategorized	Dr. Mohit Agrawal	3
Indian Institute of Technology, Kanpur (IITK)	Flow past a circular cylinder at high Reynolds numbers ~O(10square 5) will be investigated	Computational Fluid Dynamics	Dr.Sanjay Mittal	3
Institute of Nano Science and Technology (INST), Mohali.	Atomic scale design of novel nanomaterials for clean energy and devices	Computational Physics	Dr. Abir De Sarkar	9
Jamia Millia Islamia University, New Delhi.	First Principle study of the electronic structures of heterostructure devices and their related applications	Material Sciences	Dr. Anver Aziz	2
Kalinga Institute of Industrial Technology (kiit), Bhubaneswar	Estimation of Atmospheric Motion Vectors and Tropical Cyclones form Satellite Images	Uncategorized	Dr. Monideepa Roy	2
Kurukshetra University, Kurukshetra	Simulations of rare earth free magnetic inorganic halide perovskites for photovoltaic applications, Academic	Computational Physics	Dr. Manish Kumar Kashyap	4

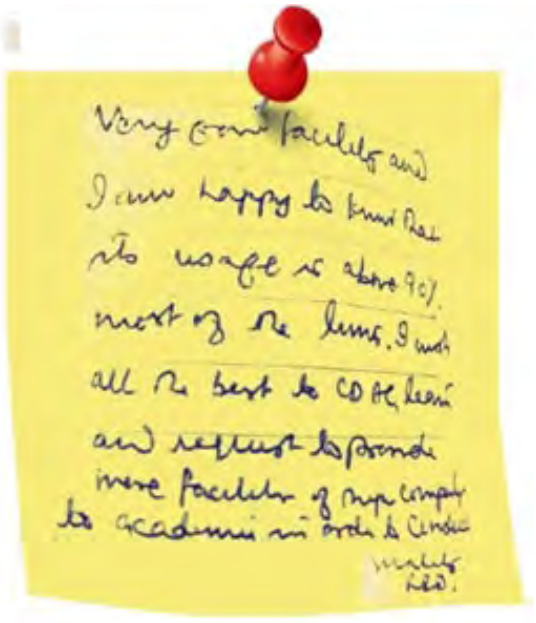
National Institute of Technology (NIT), Silchar.	Spectral element methods for elliptic and parabolic interface problems	Uncategorized	Dr. Pankaj Biswas	2

Table 1 – Continued from previous page

Institute	Project	Research Field	Chief Investigator	No. of users
Periyar University,Salem	Molecular dynamics simulation of RdRp -ligand complexe	Uncategorized	Dr. P. Kumaradhas	2
	Molecular dynamics simulation of ACE2-ligand complexes	Uncategorized	Dr. P. Kumaradhas	1
Regional Centre for Biotechnology,Faridabad	QM/MM study of enzymatic reaction mechanism	Uncategorized	Dr. Kinshuk Raj Srivastava	2
Sri Guru Granth Sahib World University,Fatehgarh Sahib	Design, Synthesis and Evaluation of Modified Short Peptides as Inhibitors of Amyloid-B (AB) Peptide Aggregation	Chemical Sciences	Dr. Deepti Goyal	5
University of Kashmir, Srinagar	Boron based Molecular Probes for Anion recognition and their Mechanism Demonstration	Chemical Sciences	Dr. Aijaz Ahmad Dar	2
University of Madras, Chennai.	Studies on hybrid organic−inorganic Halide Perovskite using first-principles density functional theory	Computational Sciences	Dr. R. Radhakrishnan	1
Women's College, Agartala	Electronic structure calculations of semiconductors	Computational Physics	Dr. Subrata Deb	1

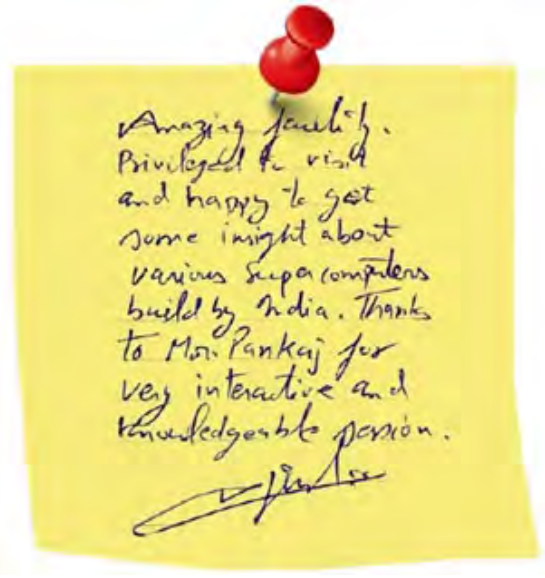
*Uncategorized: Projects for which no information on research field was provided by their respective Chief Investigators

‘E’ Quotes by Dignitaries & Visitors



Dr. Santosh K Pandey,
Sc.D/Joint Director, MeitY, Delhi

Mr. Pankaj Mishra, Survey of India,
Dehradun



DY Comdt AS Rathi, MTI (IMD)

Mr. Sanjit Choudhary

Anuradha Anil Ambedkar

‘F’ Appreciations by NPSF Users

“PARAM Yuva II has helped me immensely in guiding my Ph.D. students on a wide range of research problems. 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 Yuva II. CDAC, Pune has been doing a wonderful job for many years in helping Computational Scientists across India in their active pursuit of research. The strong computational support provided by CDAC-Pune enables us to pursue good quality research. I would like to appeal to the Govt. of India to allocate substantial funds to CDAC-Pune to support the latter in their future endeavors, which includes upgrading their HPC systems. Any HPC system gets outdated in five years. Moreover, the usage of Param Yuva II is really high. Param Yuva II caters to users from all over India. CDAC-Pune is in dire need of a strong funding support from the Govt. of India. Integration of the latest computational resources into the current HPC system is the crying need of the hour.”

Prof. Abir De Sarkar, Professor (Scientist -F)
Institute of Nano Science and Technology, Mohali

“Establishing an adequate number of high-performance computing (HPC) facilities is vital for the progress of research and technology in our country. CDAC has been working tirelessly to make superior computing resources available to scientists in our country. However, as per Moore’s law, the HPC facilities would become obsolete if not upgraded every few years. Therefore, substantial funding from the government is essential for CDAC to upgrade existing facilities and establish new ones. Hence, we request the government to support CDAC in their mission by providing better financial support.”

Dr. Achintya Kumar Dutta, Assistant Professor
Indian Institute of Technology (IIT), Bombay

“I want whole heartedly to thank CDAC staff for their timely support to resolve any technical issues faced. I immensely thank CDAC for the computational facility.”

Dr. Malay K Rana, Assistant Professor
Indian Institute of Science Education and Research (IISER), Berhampur

“National PARAM Super-computing Facility (NPSF) is a great support for the institution having insufficient computing facility. The managing team of C-DAC provides us a great support. The only difficulty I face with NPSF is that the number of cores available are very limited and one has to wait very long to get the job running. If there will be an improvement in the above limitation it will be of great help to produce more publications. Still I would say it is an excellent support!”

Dr. Sunita Patel, Visiting Scientist-II
UM-DAE Centre for Excellence in Basic Sciences, Mumbai.

"Our research group is very much greatful to the NPSF for providing the computational facilities in support of our projects. Solving the technical queries from time to time is also highly appreciated."

Prof. Mrinalini D. Deshpande, Professor, Vice Principal
H.P.T Arts and R.Y.K. Science College, Nasik

"The service is superb. I am very happy to be a part of it. Thanks to admin for providing me an opportunity to work in this pioneer field."

Dr. Subrata Deb, Assistant Professor
Women's College, Agartala

"Our work has also been highlighted on the cover page of the journal. I have acknowledged CDAC for computational resources. I want to express my gratitude for all the support I received from CDAC and I hope that we can continue to have your support to use CDAC resources"

Dr. Vijay Kumar, Founder
Dr .Vijay Kumar Foundation, Gurgaon

‘G’ Picture Gallery

Visit to NPSF by Dr. Santosh K. Pandey, Scientist C, MeitY.

Visit to NPSF by College Students on National Science Day

PARAM Siddhi-AI System Installation at NPSF

PARAM Siddhi-AI System Installation at NPSF

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बंगलुरू | चेन्नई | हैदराबाद | कोलकाता | मोहाली | मुंबई
नई दिल्ली | नोयडा | पटना | पुणे (मुख्यालय) | सिलचर | तिरुवनंतपुरम