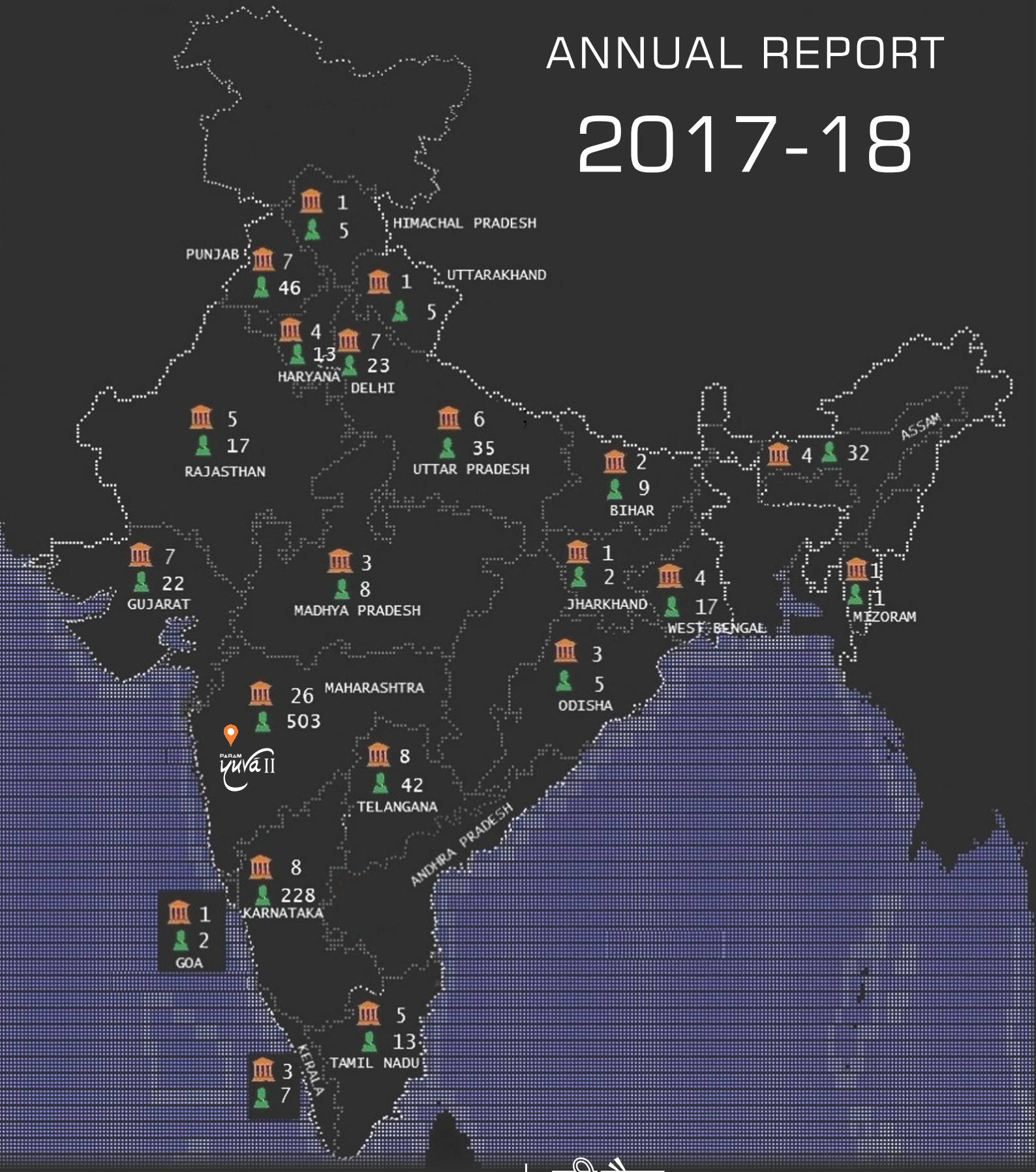
[root@npsf ~]$ National PARAM Supercomputing Facility

# ANNUAL REPORT 2017-18




NPSF National PARAM Supercomputing Facility | सी डैक CDAC

CENTRE FOR DEVELOPMENT OF ADVANCED COMPUTING

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# Message from Director General

The year 2018 is memorable Year for C-DAC as National SuperComputing Facility (NPSF) achieved a milestone of "Two Decades" of operations since its inception. Under the umbrella of NPSF, Generations of PARAM Series of Super-Computers are dedicated to the Nation. This includes PARAM 8000, PARAM 9000, PARAM 10000, PARAM Yuva and PARAM Yuva II systems. PARAM Yuva II is the current system has processed over 2.6+ lakhs of HPC jobs from 100+ Institutions with 1000+ HPC users.

With the experience and learnings, C-DAC is successful in rolling out PARAM Shavak- A smaller version of PARAM to reach up to gross root level including Engineering colleges and various R&D organizations.

I would like to take this opportunity to thank all users of NPSF for their continuous support and their excellent contribution to the Academic and Scientific community of India. These achievements enabling C-DAC to take up new challenges in the Area of High Performance Computing. Through National SuperComputing Mission (NSM), C-DAC is committed to build and deploy few HPC systems at some of the premier institutions for the benefit of HPC user community.

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

I wish you all the success for your future endeavours!

**Dr. Hemant Darbari**
**Director General, C-DAC**

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# Message from Head of Department

I feel proud to release NPSF Annual Report. This report is indeed a treasure showcasing the scientific work carried out in our Nation by various Scientific, R & D and Academic Institutions.

I congratulate NPSF team for their tireless and unrelenting contribution in supporting to over 1000+ users from 100+ R&D and academic institutions who are using NPSF facility. These highlights are just a sampling of the wealth of stories and information contained in this 2018 Annual Report. Apart from Publications, this year we are also including some of the good work being carried out using NPSF.

We hope that you will enjoy the glimpse of our recent activities. With the focus on National Supercomputing Mission (NSM), the user base is expected to grow by leaps and bounds which may need trained manpower to effectively manage the HPC systems. To cater this need, NPSF with its earned expertise of over more than two decades has started providing training on HPC administration. One of such key activity is a 15 days training to NTRO delegates on "Introduction to HPC". NPSF team is also contributing in delivering lectures on various HPC sub-areas like Schedulers, Storage etc. in DHPCA course conducted by ACTS, C-DAC.

I wish all stake holders and users who have been associated with NPSF a very productive and happy COMPUTING year ahead.

**Vinodh Kumar M.**
**Center Head, C-DAC Mohali &**
**Senior Director & HoD, HPC-I&E, C-DAC, Pune**

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# Contents

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# 1

# About NPSF

**Clusters at NPSF**

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

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

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

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

The supercomputing initiatives PARAM 10000, PARAM Yuva and PARAM Yuva II at National PARAM Supercomputing Facility has contributed to the proliferation of parallel and distribute processing technologies in India which in turn has helped several researchers from various scientific and engineering disciplines to carry out their research more effectively.

## 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 $69^{th}$ in the Top500 list released in November 2008 at the Supercomputing Conference in Austin, Texas, United States.

## PARAM 10000

PARAM 10000 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. Exported to Russia and Singapore.

## Technical Affiliation Scheme of NPSF

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

# 2

# Year 2017 - 2018 in Review

This year, NPSF ventured into providing training on various verticals of HPC. Under this, a 15 Day training was conducted for **National Technical Research Organization (NTRO)** on *Introduction to HPC* from 20th Nov, 2017 to 8th Dec, 2017.

1. NPSF HPC services were affected due failure in electrical infrastructure on **19th May 2017**. This resulted in complete shutdown of HPC system, terminating all running jobs. Services were restored on **22nd May at 1100 Hrs**.

2. **Ms. Nisha Agrawal and Shraddha Jani** carried out preliminary research work titled *Memory Bandwidth analysis of 2nd Generation Intel Xeon Phi Processor (Knights Landing) and Intel Xeon (Broadwell) Processor*. This work submitted in the form of Poster got accepted in **Women in HPC** at **ISC 2017 Conference, Frankfurt, Germany**.

3. This year, NPSF ventured into providing training on various verticals of HPC. Under this, a 15 Day training was conducted for **National Technical Research Organization (NTRO)** on *Introduction to HPC* from 20th Nov, 2017 to 8th Dec, 2017. Training program covered following topics: **MPI; OpenMP; OpenCL; CUDA; Bigdata Analytics; Cluster commissioning and administration; Image Processing.**

NPSF members and participants from NTRO

4 In continuation, NPSF team members engaged 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 6 month, twice in a year activity.

5 As an effort to apprise Chief Investigators (CI) of projects in NPSF, and also to serve as usage charges levied (not commercial), from this year onwards, NPSF has started raising invoices for monthly CPU time utilization. It is also planned to send quarterly usage statements to head of the respective institute. One such sample invoice is given below

**NATIONAL PARAM SUPERCOMPUTING FACILITY**
**Center for Development of Advanced Computing**
**Pune, India**

INVOICE No.: NPSF/2018/01/01 Date: 25-Jan-2018

**Bill to:**

**Chief Investigator of the Project:** Project Guide

**Institute:** Institute name

**Address :** Institute Full Address

**Project Name:** Project-Name-PR

**Bill Duration:** 01/12/2017 to 31/12/2017

CPU Time* consumed

**XXXXX**
(In CPU Hrs.)

**Project Account Monthly Summary For December-2017**

| Opening CPU Time Balance | Credited CPU Time | Total CPU Time Amount | CPU Time Consumed | Closing CPU Time Balance |
|---|---|---|---|---|
| xxxxxxx | xxxx | xxxxxxx | xxxxx | xxxxxxx |

Above figures are in CPU Hours

**No. of Jobs processed: xx**

eMoney† consumed

**XXX**
Debit Points‡

(This is a computer generated invoice and no signature is required.)
**Authorized Signatory**

*CPU Time = No. of CPU Cores x No. of Hours consumed.

†eMoney = CPU Time x INR 3.00/hour.

‡One Debit Point is equivalent to 1000 INR.

6 On 4th Jan, 2018, **Mr. Y. S. Swarup** delivered invited talk on *Overview of PARAM Yuva II"* at MIT WPU Kothrud, Pune.

7 On February 16, 2018, **Ms. Nisha Agrawal** delivered invited talk on *MPI Programming* for faculties and students of Pune Institute of Computer Technology (PICT), Pune.

8 As part of C-DAC's tradition, NPSF team participated to showcase highlights of activities related to NPSF during National Science Day celebration at C-DAC, Pune, which this year fell on February 28, 2018. PARAM Yuva II model display attracted most attention by school student and general public alike. In total, around 1600 visitors (Students from various colleges and schools) from Pune and nearby districts like Mumbai enjoyed the technical sessions and walk-through of NPSF.

NPSF volunteers in National Science Day event, C-DAC, Pune.

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# 3

# Insights

Total compute nodes 290 (221 nodes of PARAM Yuva II + some preserved old nodes).

PARAM Yuva II compute node is equipped with two no. of Intel Xeon Phi 5110P accelerator. Each such accelerator is having 61 CPU cores and delivers 1 TF.

More than 50 open source scientific applications/libraries/tools made available.

| **Three Subclusters** | |
|---|---|
| Subcluster-1 | **PARAM Yuva II:**<br>221 nodes cluster of Intel server system R2000GZ with<br>Dual socket Intel Xeon E5 2670 (Sandy Bridge) Processor per node<br>Eight CPU cores per socket, 2.6 GHz<br>Two Intel Xeon Phi 5110P per node<br>Infiniband FDR interconnect<br>Partitions: TESTp, FDRp, BIGJOBp, SDSp |
| Subcluster-2 | 60+ nodes cluster of HP Proliant DL580 G5 with<br>Quad socket Intel Xeon X7350 Processor per node<br>Four CPU cores per socket, 2.93 GHz<br>System interconnects: PARAMNet3, Infiniband DDR<br>Partition: DDRp |

| | |
|---|---|
| Subcluster-3 | Four nodes cluster of Supermicro SuperServer 1027GR-TRF with<br>Dual socket Intel Xeon E5 2650 (Sandy Bridge) Processor per node<br>Eight CPU cores per socket, 2.6 GHz<br>Two NVIDIA GPU Tesla M2090 per node<br>Infiniband FDR interconnect<br>Partition: GPUp |
| **Storage** | PFS based scratch space with 10 GB/s write bandwidth<br>User Home Area: 178TB<br>Archival: 800TB |
| **Software** | Operating System: CentOS v6.2, Kernel v2.6.32-220<br>Intel Cluster Studio XE 2013<br>Intel Cluster Studio XE 2015<br>PGI Cluster Development Kit |
| **Applications** | Libraries and software for file formats, data bases and math<br>Many scientific applications for material science/quantum chemistry, molecular modelling, computational fluid dynamics, climate modelling, circuit simulations and many more like aerospace engineering. |

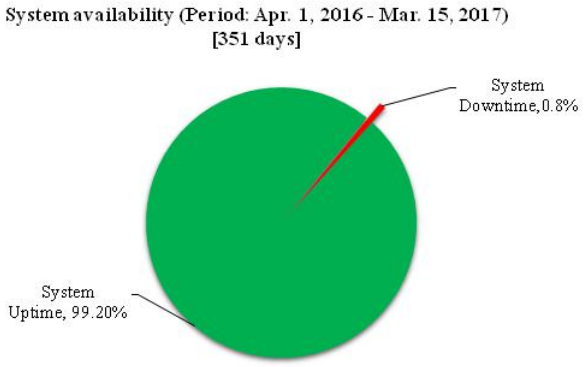
# 4

# Statistics

In Year 2017-18 : Users added : 96 ; Institution added : 16 ; Jobs Processed : 42564

## 4.1 System

### System availability



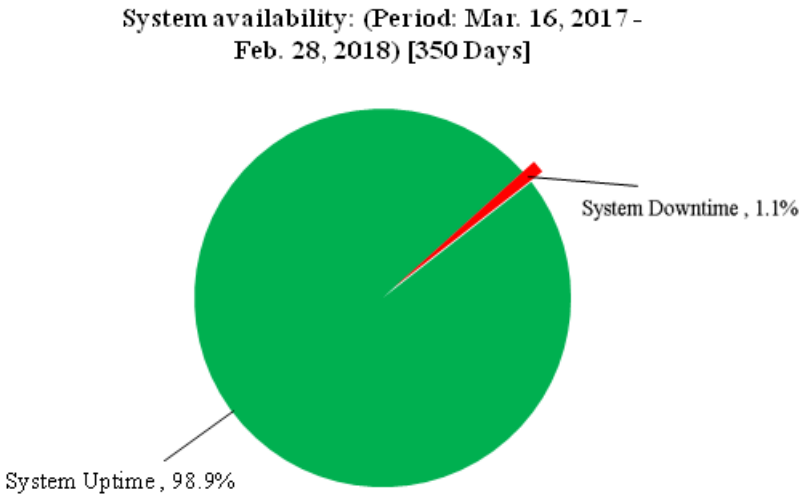
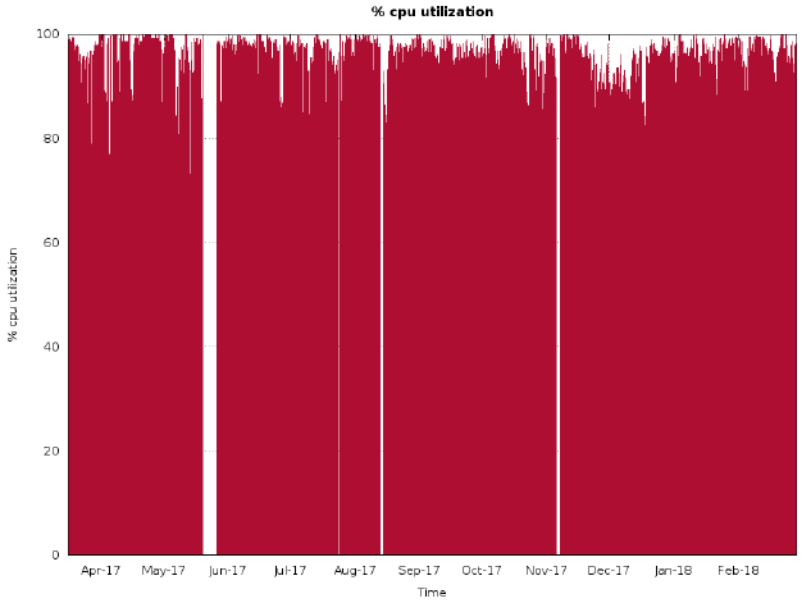



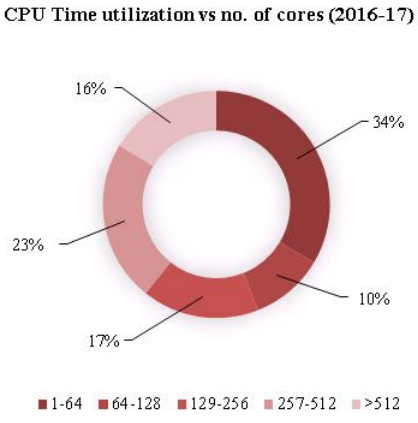
Table: System availability

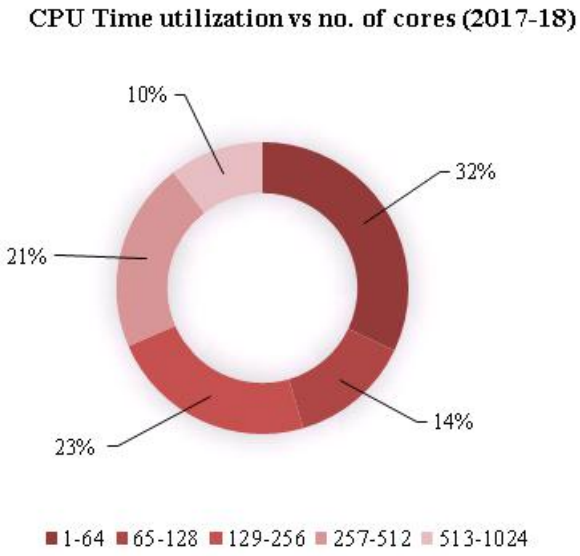
| Duration | Total Time | Downtime |
|---|---|---|
| 16Mar'17-28Feb'18 | 350 Days(total : 8400 Hours) | 3 Days, 21 Hours (total : 93Hours) |
| 1Apr16-15Mar17 | 351 Days (total : 8424 Hours) | 2 Days, 18 Hours (total : 66 Hours) |

## System utilization




## CPU time utilization w.r.t. job sizes



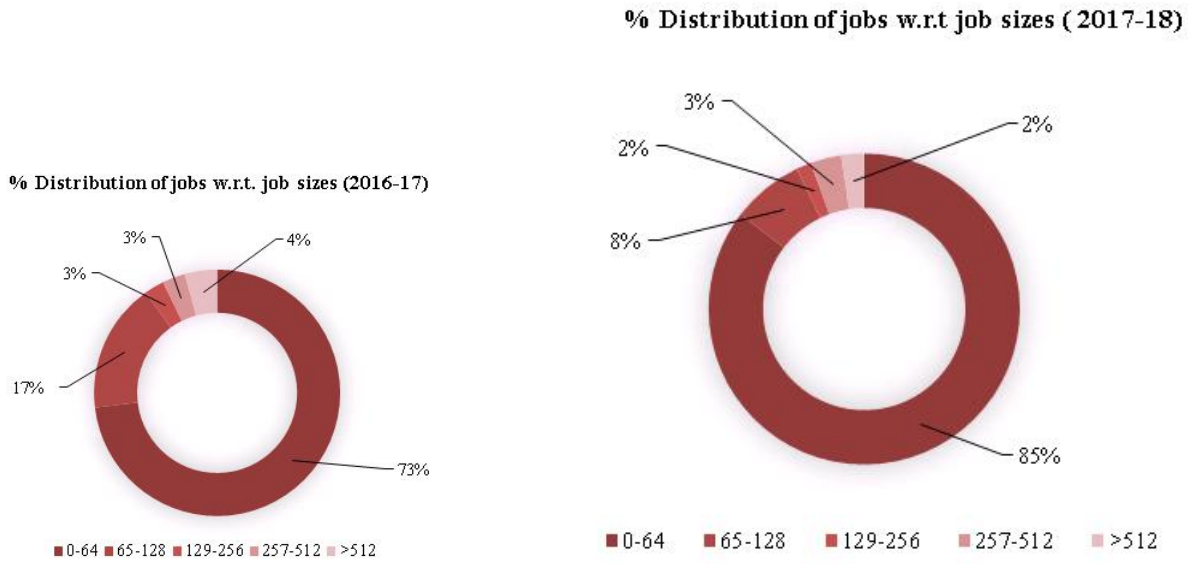




Above graph presents how allocated CPU time was consumed with respect to job sizes.

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

| | CPU time utilized (in seconds) | |
|---|---|---|
| Job Sizes | 2016-18 | 2017-18 |
| 1-64 | 40084868227 | 37931720605 |
| 65-128 | 12499978368 | 15937841856 |
| 129-256 | 19899317592 | 27205492336 |
| 257-512 | 27450739824 | 24952112240 |
| >512 | 19464235056 | 12348922448 |

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




Above graph presents % distribution of jobs across job sizes with 85% of them requesting 64 or less no. of CPU cores. This observation is complemented by % distribution queue wise. It can be noted that there is an increase of 12% from previous year for said job size and 9% decrease for 65-128.

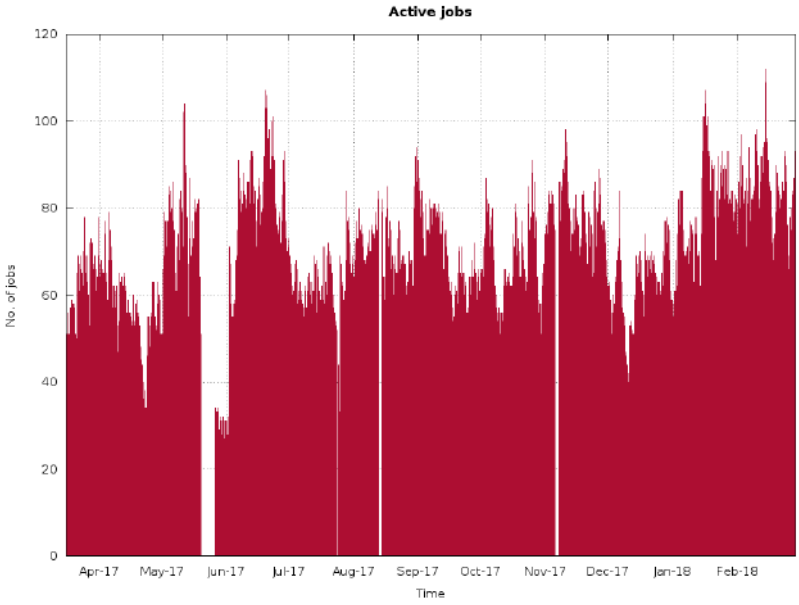
Table: Distribution of jobs w.r.t. job sizes

| | Job Count | |
|---|---|---|
| Job Sizes | 2016-17 | 2017-18 |
| 1-64 | 23560 | 36345 |
| 65-128 | 5499 | 3181 |
| 129-256 | 837 | 663 |
| 257-512 | 972 | 1366 |
| >512 | 1364 | 1009 |

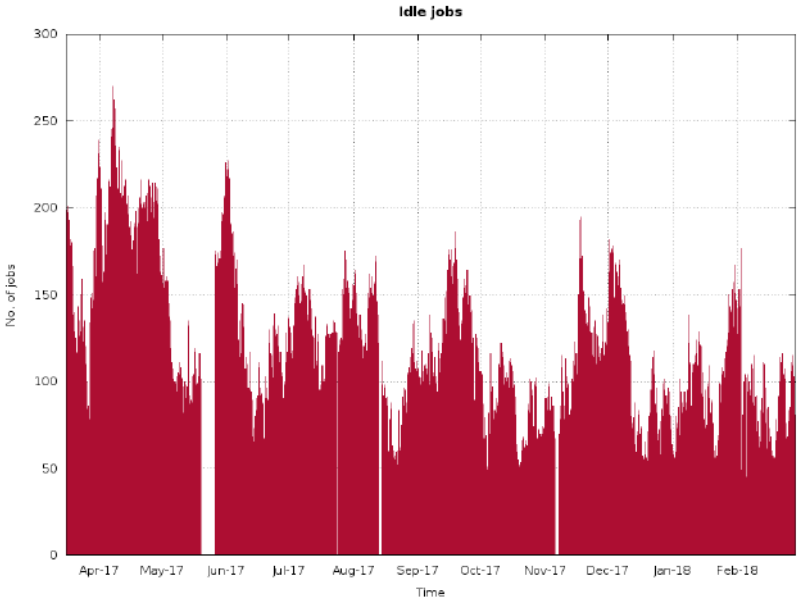
## Active jobs, idle jobs & system backlog

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 resources

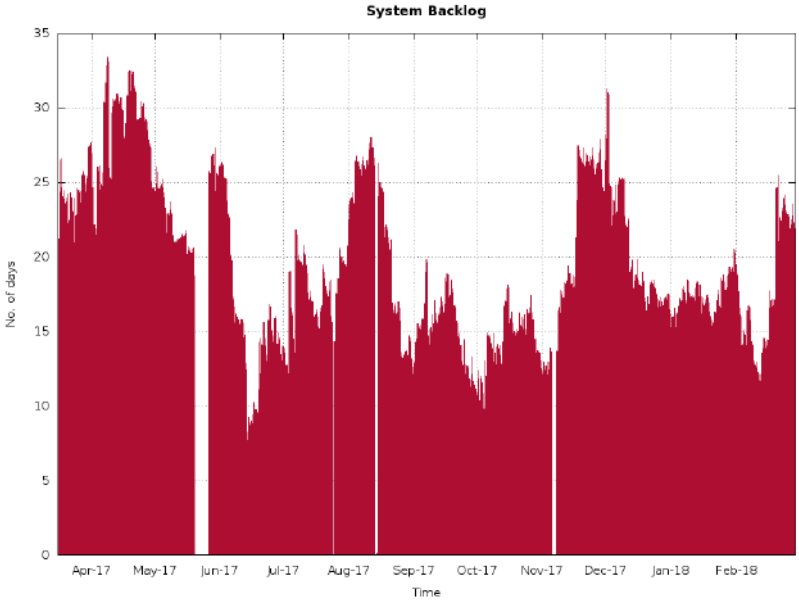
### Active jobs




### Idle jobs



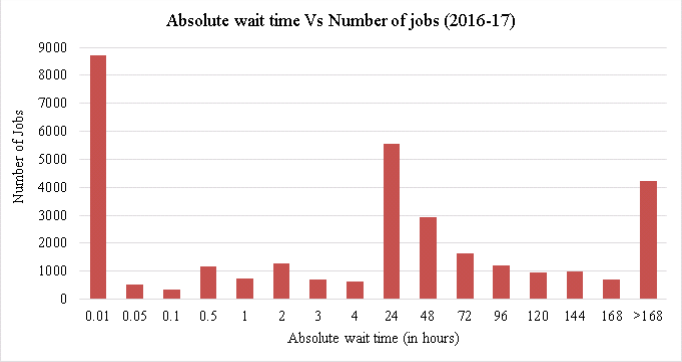
## System backlog

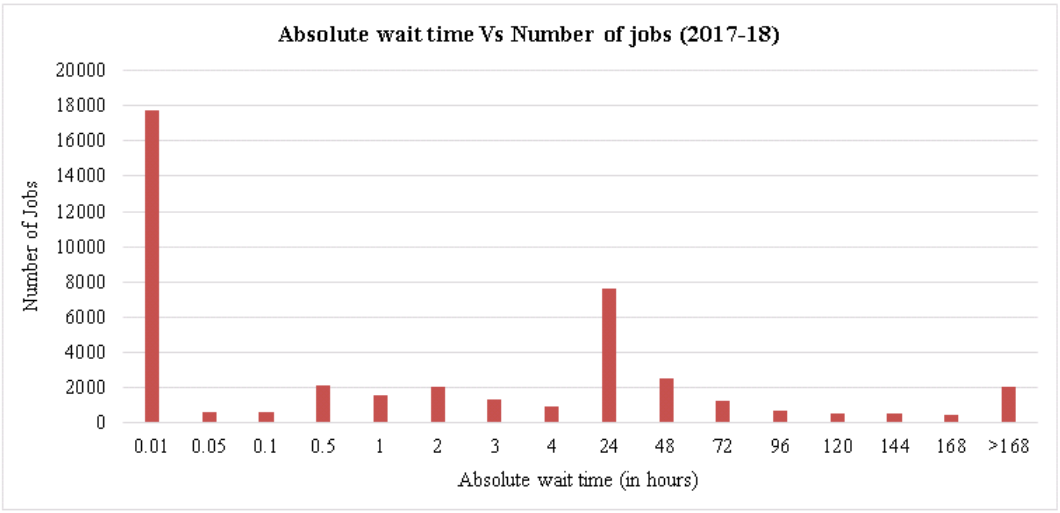



System backlog is computed as the total time required to process all idle jobs in the system, given that 1) No new jobs are introduced, & 2) State of the system is not changed, including compute capacity.

## Absolute waittime Vs no. of jobs

Absolute waittime for a job is the time spent in the queue, after submission, till allocation of resources and execution.






Above graphs shows that there is overall decrease in absolute waittime for most of the jobs. Above presentation is irrespective of job size.

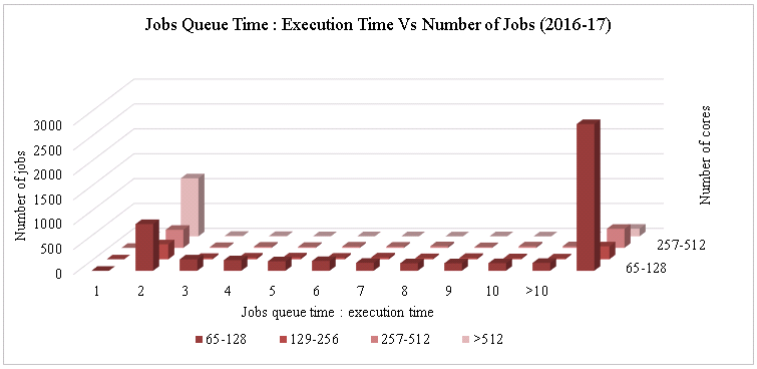
Table: Absolute waittime Vs no. of jobs

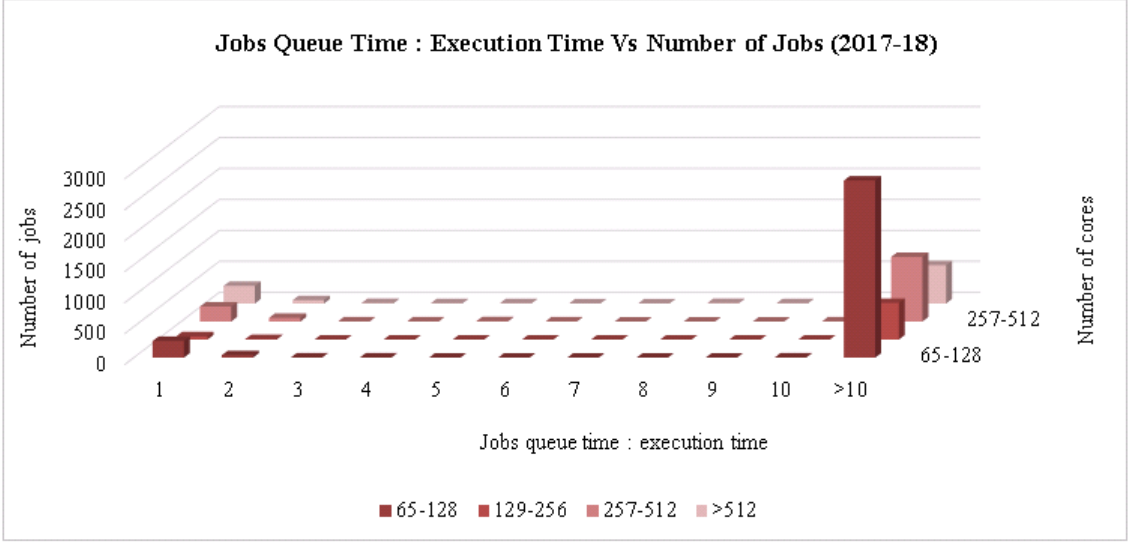
| | No. of jobs | |
|---|---|---|
| Absolute wait time (in hours) | 2016-17 | 2017-18 |
| 0.01 | 8703 | 17730 |
| 0.05 | 535 | 622 |
| 0.1 | 328 | 580 |
| 0.5 | 1180 | 2136 |
| 1 | 733 | 1538 |
| 2 | 1284 | 2075 |
| 3 | 695 | 1310 |
| 4 | 637 | 951 |
| 24 | 5546 | 7628 |
| 48 | 2918 | 2518 |
| 72 | 1633 | 1238 |
| 96 | 1218 | 702 |
| 120 | 956 | 553 |
| 144 | 1001 | 517 |
| 168 | 713 | 474 |
| >168 | 4215 | 2038 |

## 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

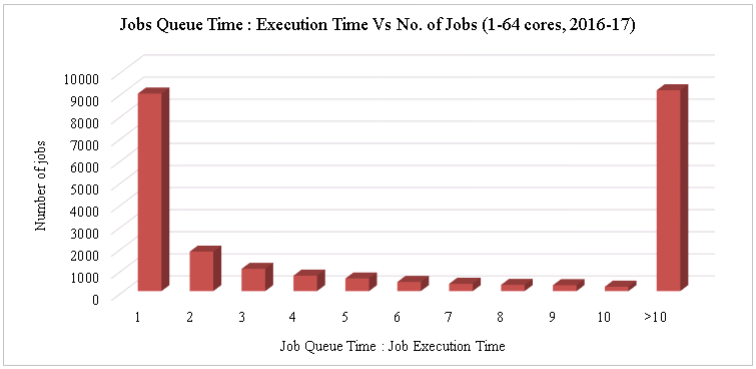
jobs and on Z-axis, jobs are binned by number of CPU cores.




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 noted that there is a remarkable increase from previous year, in jobs waiting for more than 10 times their execution time for all job sizes barring 65-128 category. This inference indicates resource crunch and impresses upon need for augmenting compute capacity.



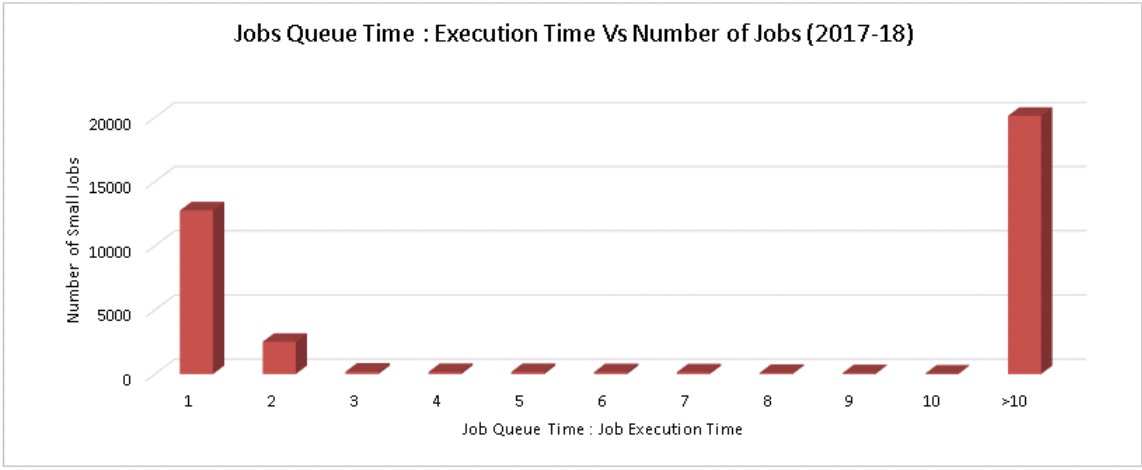



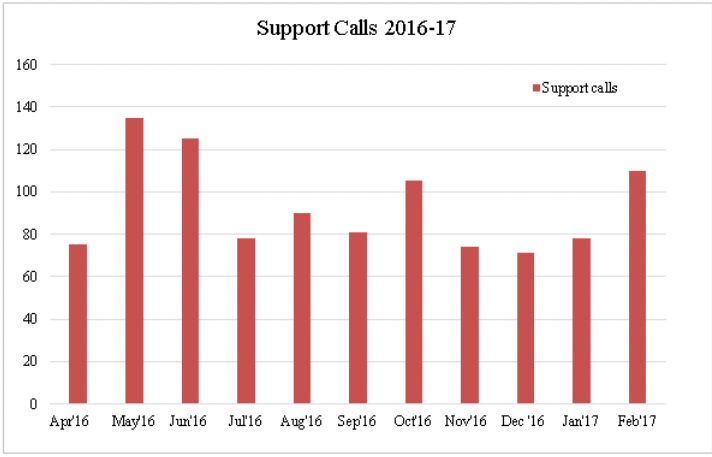

Table : Ratio of job waittime : execution time Vs number of jobs

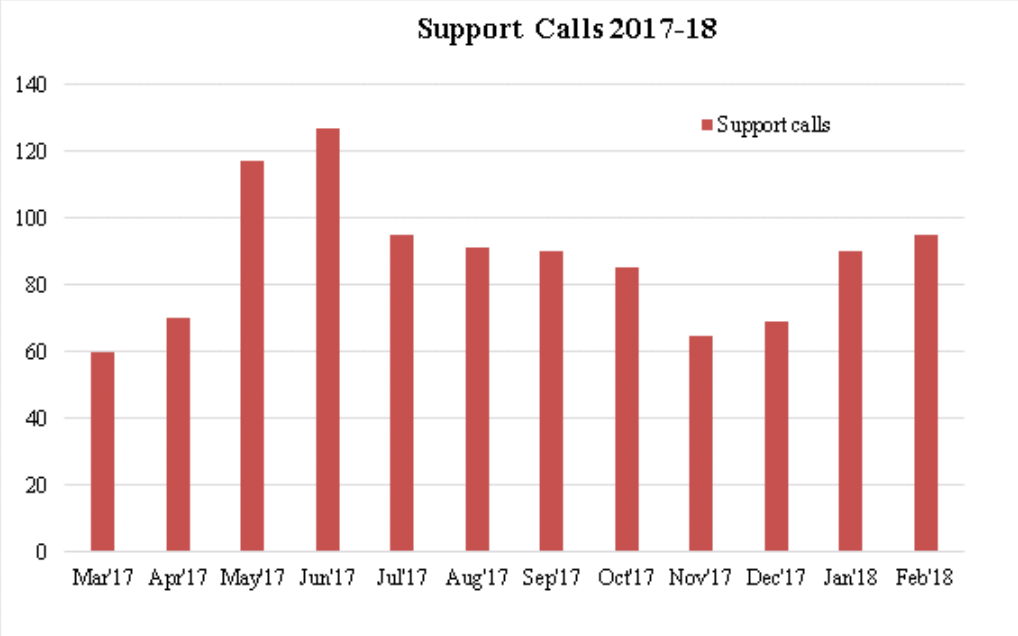
| 2016-17 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | >10 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1-64 | 8944 | 1788 | 1011 | 703 | 573 | 417 | 334 | 284 | 271 | 201 | 9095 |
| 65-128 | 940 | 230 | 213 | 191 | 198 | 161 | 151 | 151 | 153 | 159 | 2950 |
| 129-256 | 302 | 30 | 37 | 40 | 35 | 39 | 25 | 29 | 22 | 20 | 260 |
| 257-512 | 363 | 17 | 25 | 20 | 27 | 26 | 34 | 16 | 31 | 33 | 383 |
| >512 | 1168 | 12 | 8 | 5 | 4 | 4 | 0 | 3 | 1 | 2 | 155 |

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

| 2017-18 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | >10 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1-64 | 12752 | 2514 | 185 | 158 | 160 | 148 | 137 | 92 | 69 | 35 | 20123 |
| 65-128 | 270 | 40 | 5 | 5 | 2 | 2 | 2 | 0 | 1 | 4 | 2861 |
| 129-256 | 54 | 11 | 1 | 1 | 2 | 1 | 1 | 1 | 1 | 0 | 593 |
| 257-512 | 242 | 61 | 3 | 4 | 6 | 3 | 0 | 2 | 0 | 4 | 1044 |
| >512 | 285 | 56 | 10 | 6 | 6 | 3 | 4 | 8 | 5 | 7 | 619 |

### User support calls

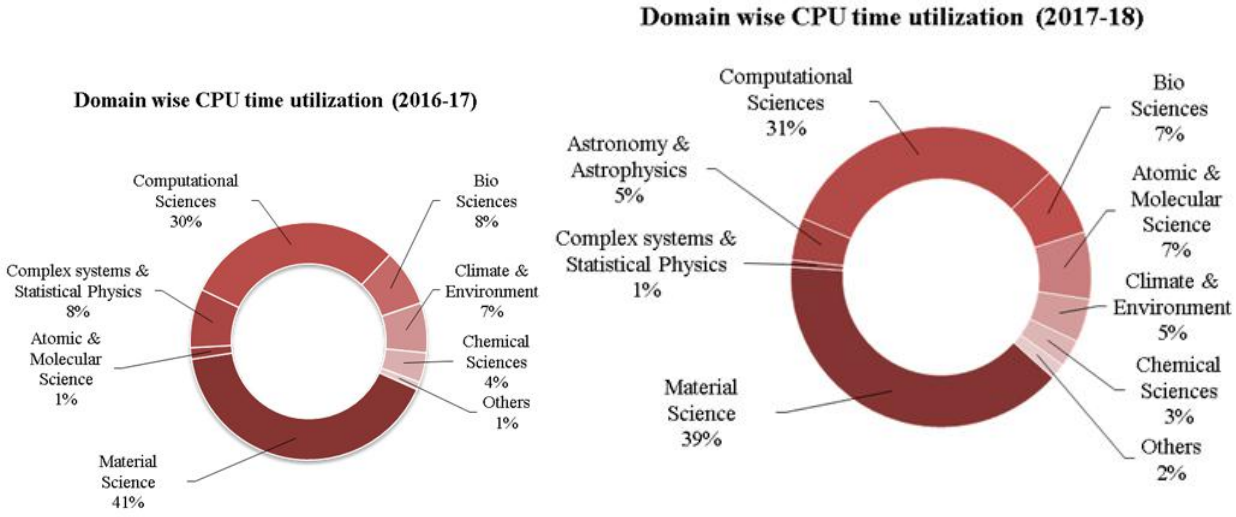



## 4.2 Domain and Institute

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

## Domain wise CPU time utilization

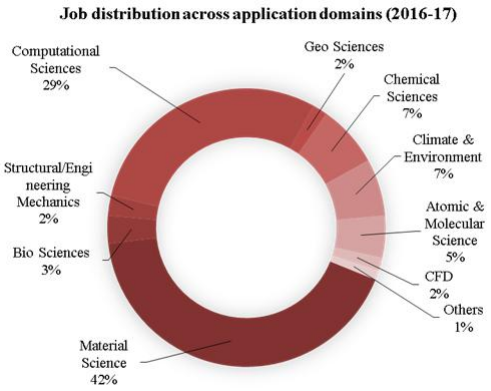


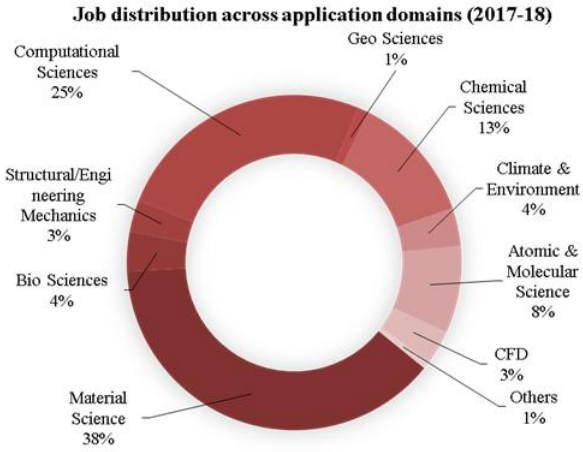

Above plots brings forth CPU time distribution across various application domains. There is a new entrant, Astronomy & Astrophysics. Usage for Atomic & Molecular Science have increased by a factor of ˜5.

Table: Domain wise CPU time utilization

| | CPU time in seconds | |
|---|---|---|
| | 2016-17 | 2017-18 |
| Material Science | 46651494317 | 47088257133 |
| Atomic & Molecular Science | 1778142694 | 8660588966 |
| Complex systems & Statistical Physics | 9151249044 | 906016828 |
| Computational Sciences | 34080912784 | 37525824164 |
| Bio Sciences | 8839738945 | 8722410029 |
| Climate & Environment | 7774204697 | 5546385762 |
| Chemical Sciences | 4628141946 | 3540023654 |
| Astronomy & Astrophysics | 0 | 5475440608 |
| Others | 1166849614 | 2008782612 |

## Job distribution across application domains



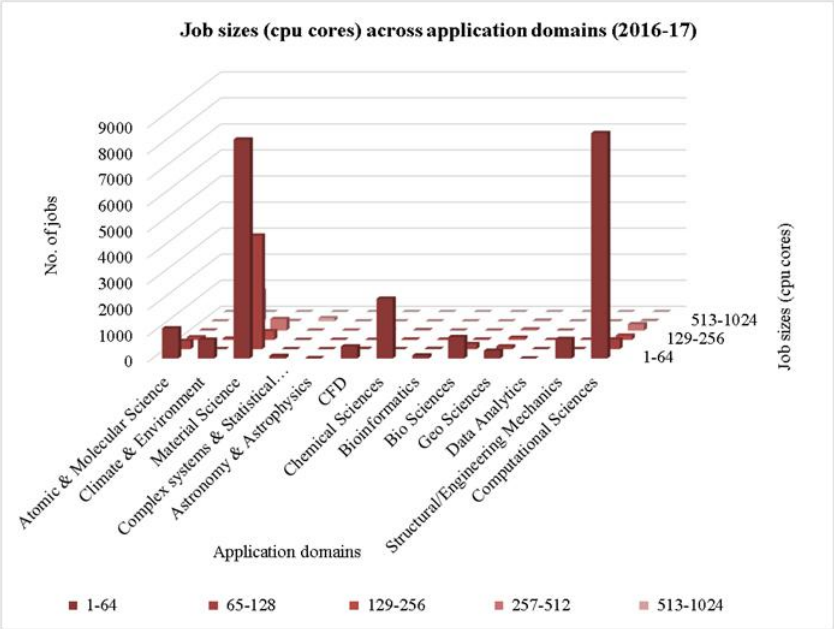




Above plots shows application domain wise percentage distribution of number of jobs processed. Apart from "Climate & Environment", it can be seen that number of jobs have increased for others.

Table:Job distribution across application domains

| | No. of Jobs | |
|---|---|---|
| Application Domain | 2016-17 | 2017-18 |
| Material Science | 13556 | 16114 |
| Bio Sciences | 1033 | 1594 |
| Structural/Engineering Mechanics | 758 | 1303 |
| Computational Sciences | 9442 | 10591 |
| Geo Sciences | 554 | 449 |
| Chemical Sciences | 2333 | 5222 |
| Climate Environment | 2135 | 1539 |
| Atomic Molecular Science | 1570 | 3534 |
| CFD | 480 | 410 |
| Others | 371 | 87 |

## Job sizes across application domain




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

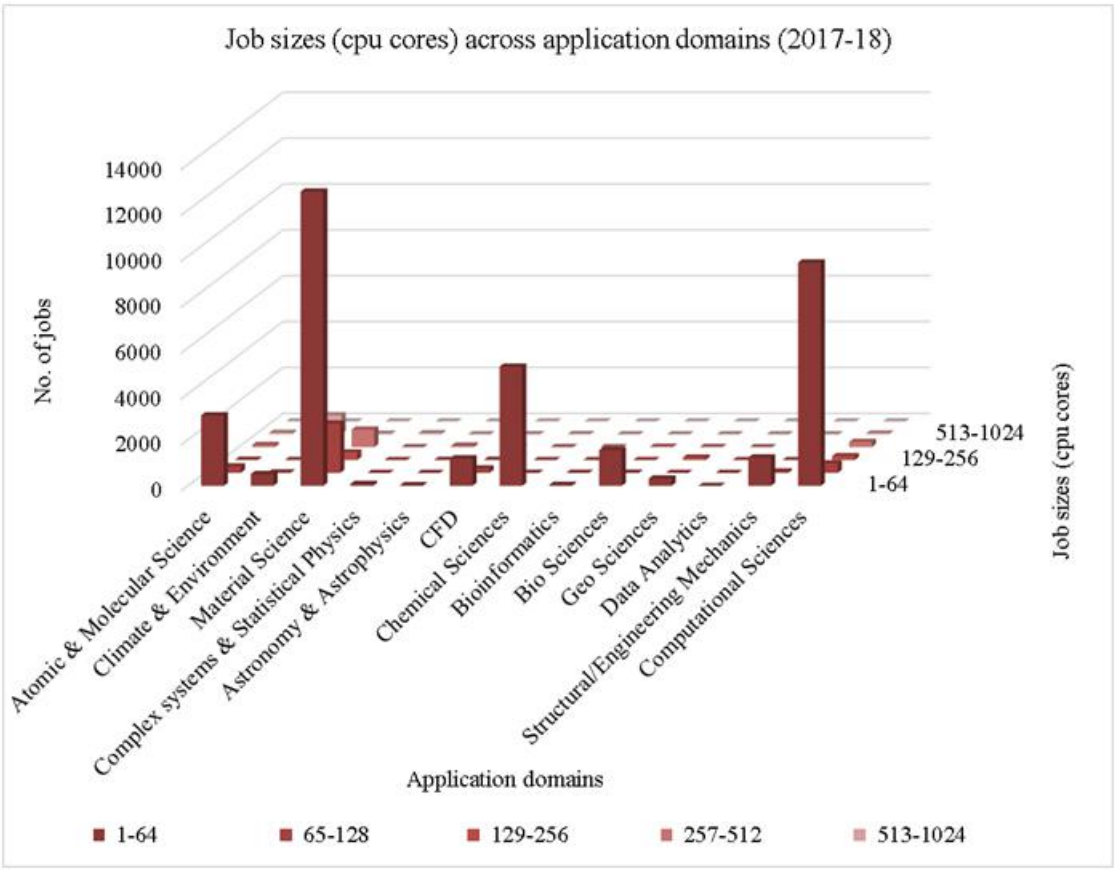


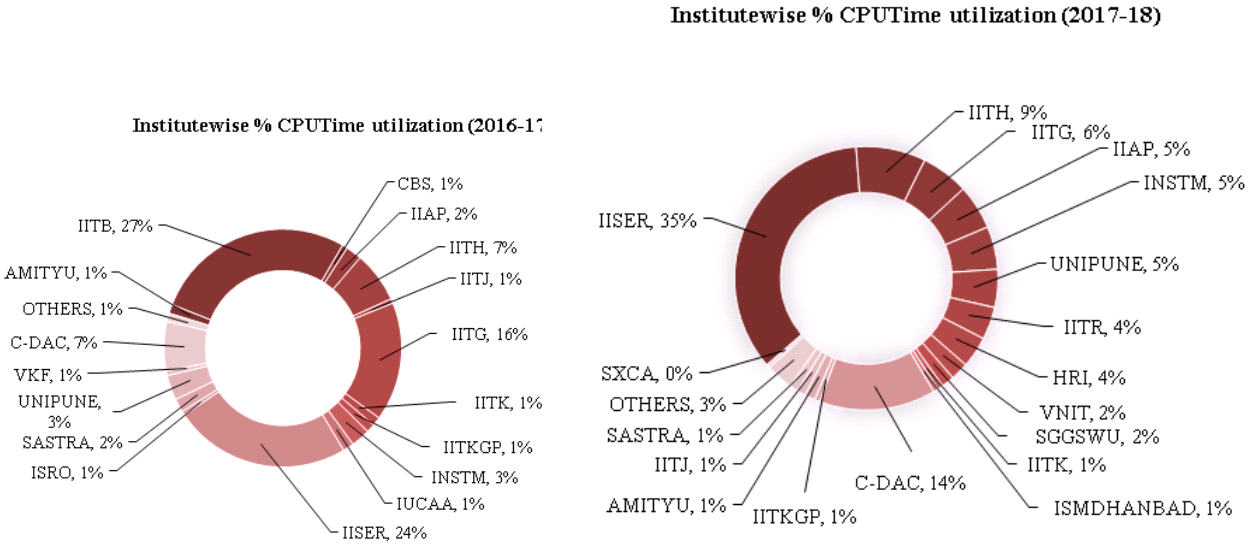
Table: Job sizes across application domain 2016-17

| 2016-17 | 1-64 | 65-128 | 129-256 | 257-512 | 513-1024 |
|---|---|---|---|---|---|
| Atomic & Molecular Science | 1156 | 314 | 97 | 3 | 0 |
| Climate & Environment | 724 | 5 | 47 | 183 | 1176 |
| Material Science | 8407 | 4359 | 334 | 444 | 12 |
| Complex systems & Statistical Physics | 99 | 0 | 0 | 0 | 120 |
| Astronomy & Astrophysics | 9 | 2 | 1 | 0 | 0 |
| CFD | 462 | 13 | 3 | 1 | 0 |
| Chemical Sciences | 2294 | 0 | 15 | 24 | 0 |
| Bioinformatics | 117 | 13 | 10 | 0 | 0 |
| Bio Sciences | 822 | 198 | 13 | 0 | 0 |
| Geo Sciences | 299 | 103 | 79 | 45 | 28 |
| Data Analytics | 0 | 0 | 0 | 0 | 0 |
| Structural/Engineering Mechanics | 748 | 5 | 5 | 0 | 0 |
| Computational Sciences | 8654 | 372 | 161 | 243 | 12 |

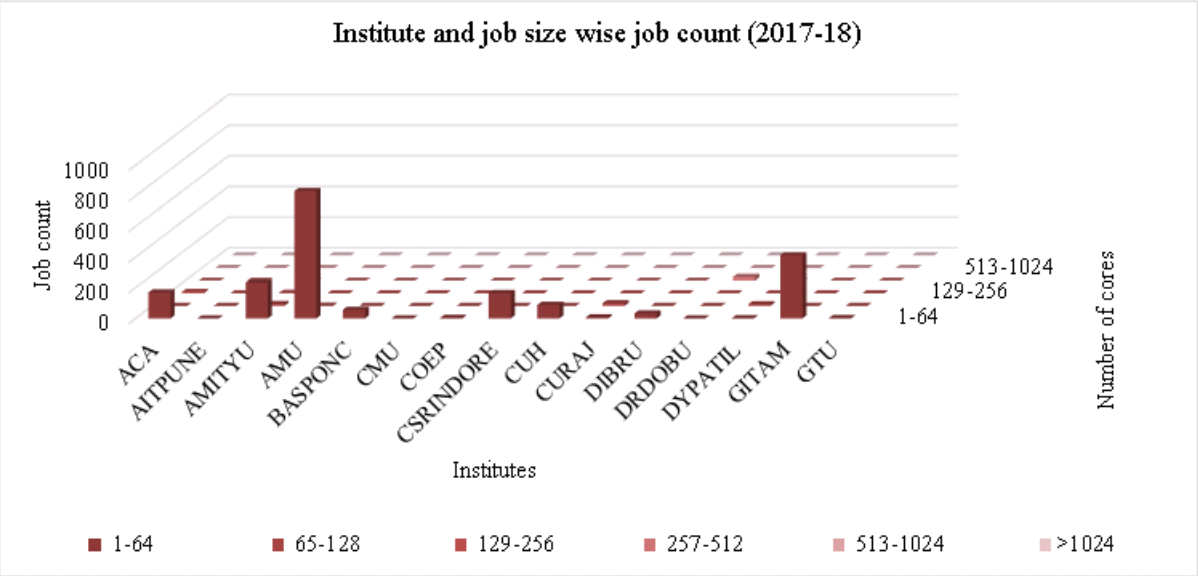
Table: Job sizes across application domain 2017-18

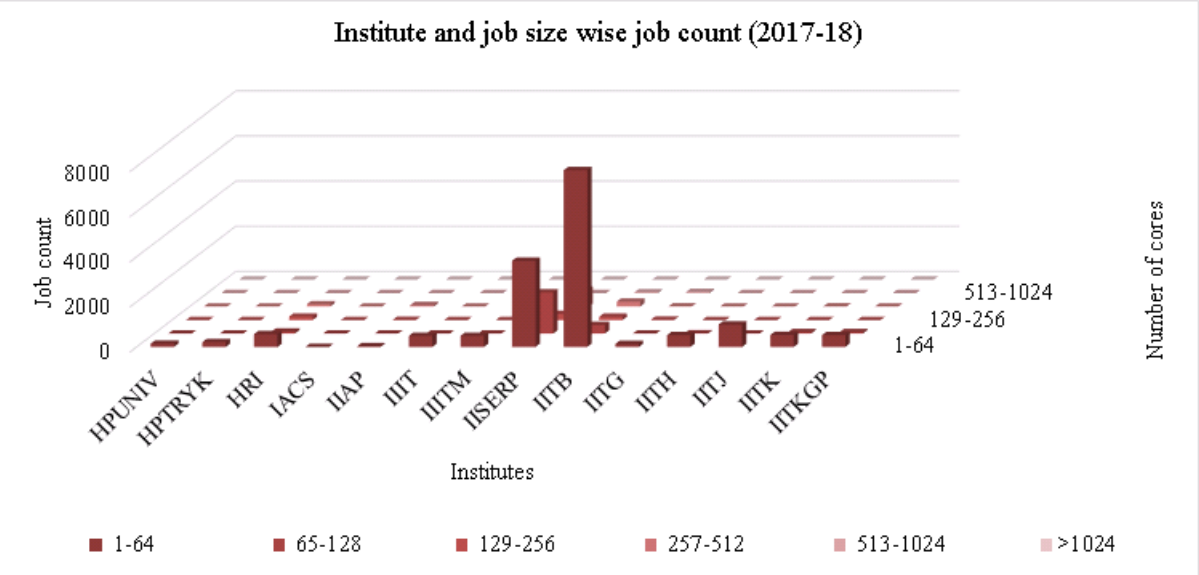
| 2017-18 | 1-64 | 65-128 | 129-256 | 257-512 | 513-1024 |
|---|---|---|---|---|---|
| Atomic & Molecular Science | 3075 | 286 | 15 | 96 | 62 |
| Climate & Environment | 515 | 26 | 6 | 162 | 830 |
| Material Science | 12828 | 2156 | 336 | 769 | 25 |
| Complex systems & Statistical Physics | 83 | 0 | 0 | 0 | 45 |
| Astronomy & Astrophysics | 32 | 1 | 7 | 67 | 0 |
| CFD | 1199 | 197 | 13 | 0 | 1 |
| Chemical Sciences | 5199 | 9 | 1 | 4 | 9 |
| Bioinformatics | 45 | 6 | 1 | 0 | 0 |
| Bio Sciences | 1557 | 11 | 1 | 25 | 0 |
| Geo Sciences | 324 | 0 | 111 | 14 | 0 |
| Data Analytics | 0 | 0 | 0 | 0 | 0 |
| Structural/Engineering Mechanics | 1239 | 62 | 1 | 1 | 0 |
| Computational Sciences | 9741 | 414 | 171 | 228 | 37 |

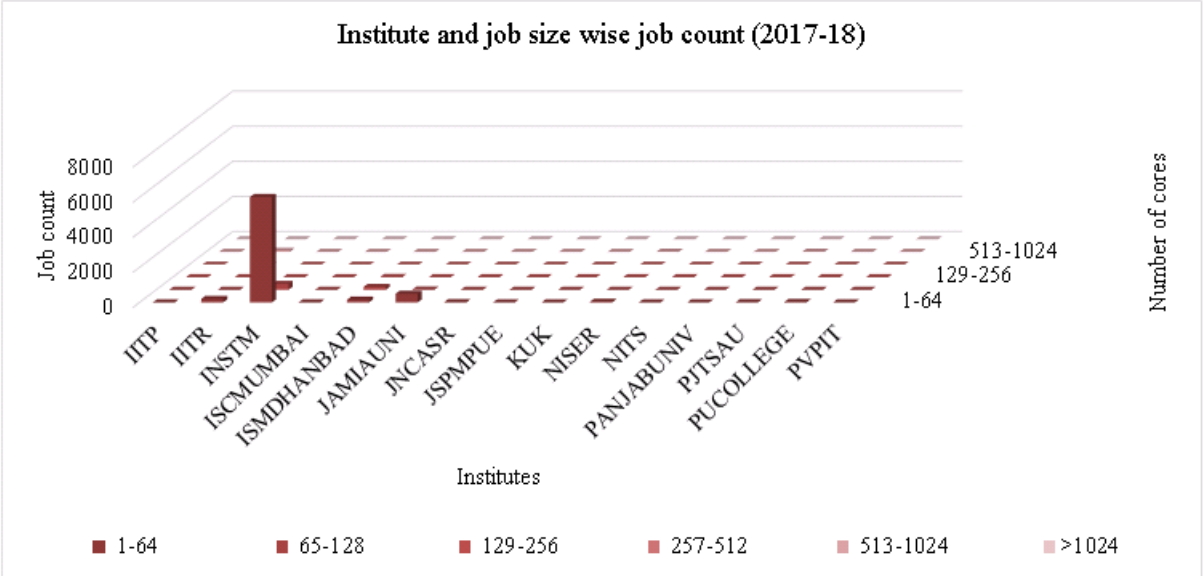
## Institute wise CPU time utilization

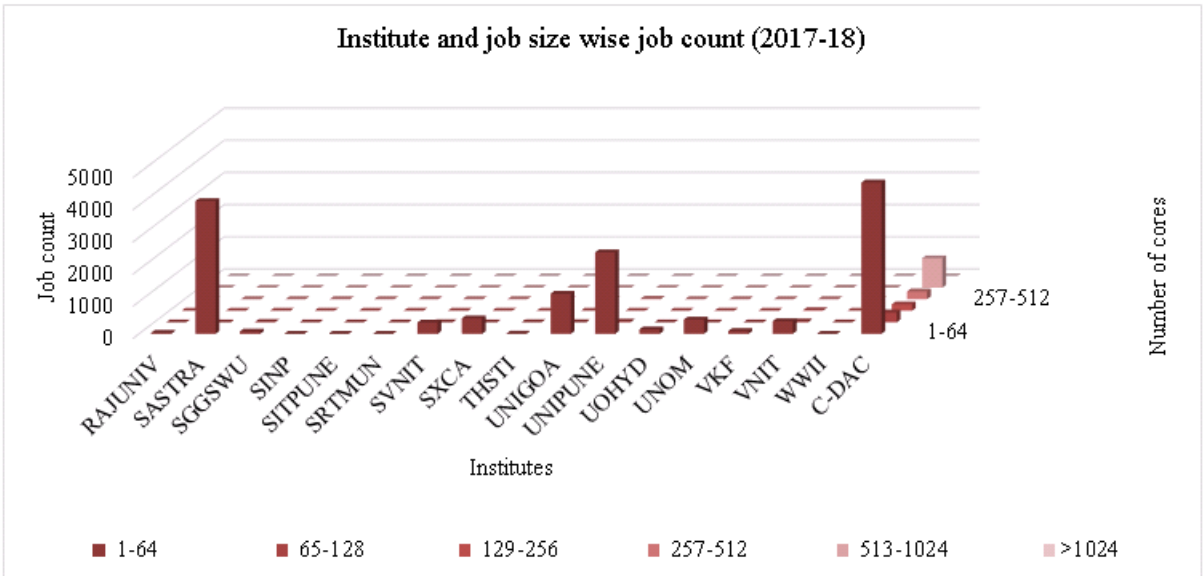



## Institute and job size wise job count




Institute and job size wise job count (2017-18)
Job count
8000
6000
4000
2000
0
HPUNIV
HPTRYK
HRI
IACS
IIAP
IIIT
IIITM
IISERP
IITB
IITG
IITH
IITJ
IITK
IITKGP
Institutes
513-1024
129-256
1-64
Number of cores
1-64
65-128
129-256
257-512
513-1024
>1024


Institute and job size wise job count (2017-18)
Job count
8000
6000
4000
2000
0
IITP
IITR
INSTM
ISCMUMBAI
ISMDHANBAD
JAMIAUNI
JNCASR
JSPMPUE
KUK
NISER
NITS
PANJABUNIV
PJTSAU
PUCOLLEGE
PVPIT
Institutes
513-1024
129-256
1-64
Number of cores
1-64
65-128
129-256
257-512
513-1024
>1024


Institute and job size wise job count (2017-18)
Job count
5000
4000
3000
2000
1000
0
RAJUNIV
SASTRA
SGGSWU
SINP
SITPUNE
SRTMUN
SVNIT
SXCA
THSTI
UNIGOA
UNIPUNE
UOHYD
UNOM
VKF
VNIT
WWII
C-DAC
Institutes
257-512
1-64
Number of cores
1-64
65-128
129-256
257-512
513-1024
>1024

## 4.3 Queue

### Job Submission Queues

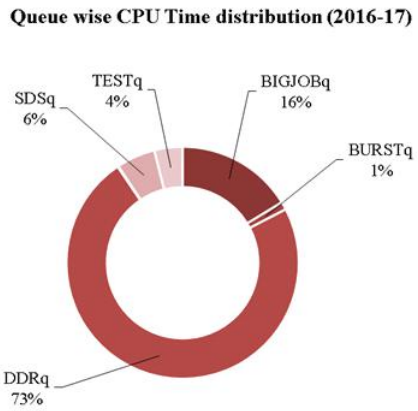
Various queues ensures a spectrum of quality of service according to the resource requirement of the users for different computing exercises. Table-4.1 shows the summary of job submission queues.

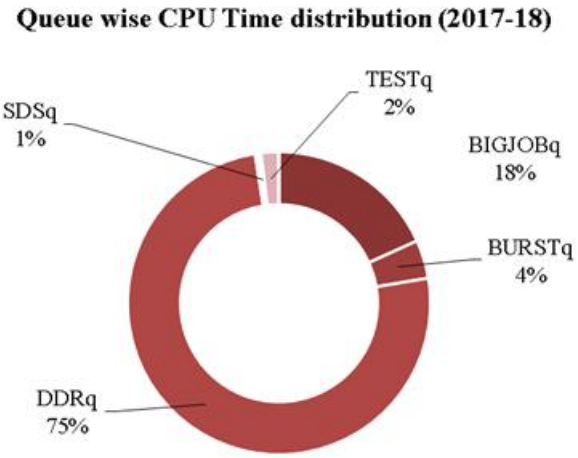
Table 4.1: Summary of queues on NPSF

| Queue | Wall Time Limit | Accelerator(s) in the nodes in the partition |
|---|---|---|
| batch | 7 Days | Xeon Phi |
| TESTq | 2 Hours | Xeon Phi |
| GPUq | 7 Days | GPU |
| SDSq | 06 Hours | Xeon Phi |
| BURSTq | 17 Hours 55 Minutes | Xeon Phi |

- TESTq: The users get resources without having to wait longer to run the test jobs before the actual job runs. Currently the maximum allowed walltime for TESTq queue is 2 Hrs per job.
- GPUq: Queue for jobs with GPU nodes/SMP node.
- SDSq: Queue for jobs on resources with advanced reservation. The resources in under SDSq are primarily for running the production jobs on daily basis for a fixed duration as per the commitment to different users.
- BURSTq: Queue for jobs requiring large number of cores for less wall time.

### % Distribution of CPU time utilization w.r.t. Job queues



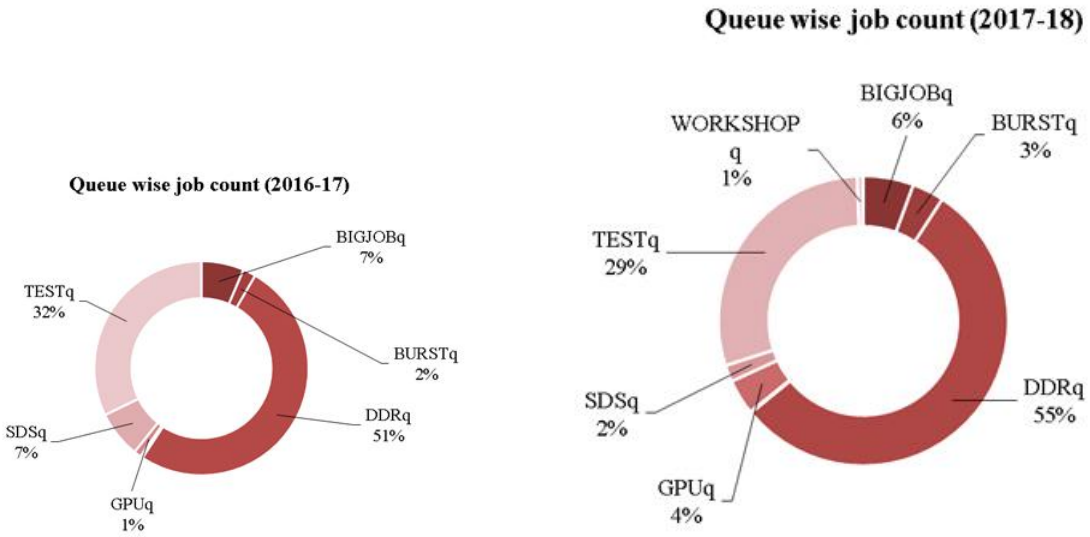
Above graph shows distribution in percentage of CPU time utilized by jobs in respective queues. DDRq and BIGJOBq accounts for ˜90% of usage with former leads.

**Note** : Percentage CPU time utilization of WORKSHOPq not presented owing to less utilization and scale.

Table: Distribution of CPU time utilized by jobs

| | CPU Hours | |
|---|---|---|
| Queue | 2016-17 | 2017-18 |
| BIGJOBq | 27735366438 | 39607197720 |
| BURSTq | 1857597056 | 8902900224 |
| DDRq | 1.24652E+11 | 1.63083E+11 |
| FDRq | 47360 | 15204 |
| GPUq | 179382368 | 588302112 |
| SDSq | 9221228808 | 769674332 |
| TESTq | 6676972900 | 4124914568 |
| WORKSHOPq | 27735366438 | 946974 |

## % Distribution of job counts w.r.t. queues

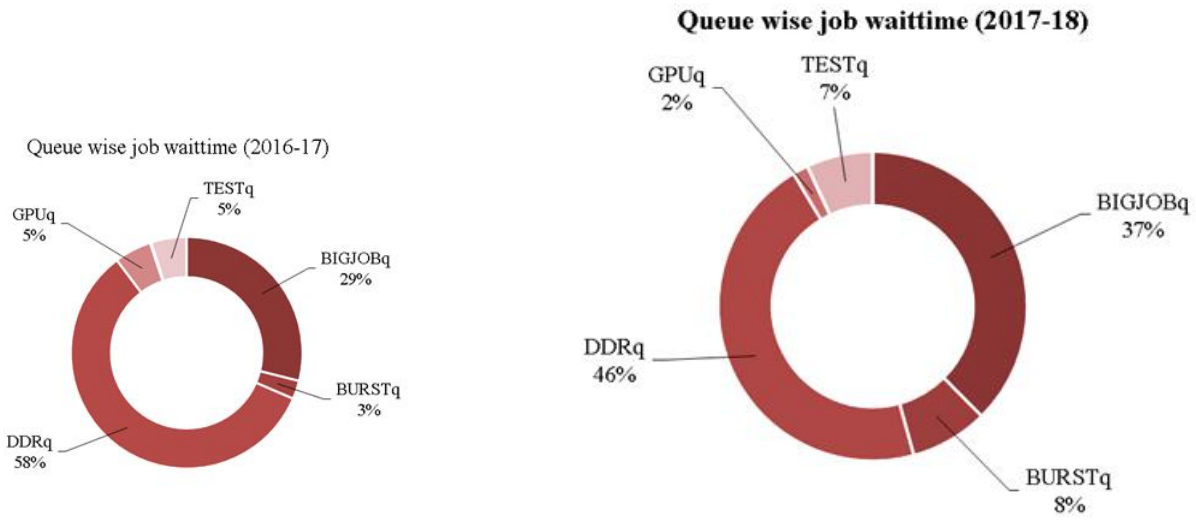



Above graph shows distribution in percentage of jobs among execution queues. It is observed that majority of jobs were directed to DDRq, relating to fact that for 55% of total executions, job size was below 65 CPU cores.

Table: Distribution of jobs among execution queues

| | Job count | |
|---|---|---|
| Queue | 2016-17 | 2017-18 |
| BIGJOBq | 2069 | 2390 |
| BURSTq | 628 | 1513 |
| DDRq | 16405 | 23370 |
| FDRq | 117 | 61 |
| GPUq | 354 | 1675 |
| SDSq | 2284 | 787 |
| TESTq | 10375 | 12477 |

## % Distribution of job wait time w.r.t.queues




Above graph is a representation of percentage distribution of time spent by jobs, once submitted, until allowed for execution on system. Due to restriction of maximum walltime for a job as per policy, jobs submitted to TESTq experience least wait. Wait time for jobs in DDRq is the largest, owing to 55% of total job submissions. Please note, calculation of waittime is irrespective of CPU cores requested.

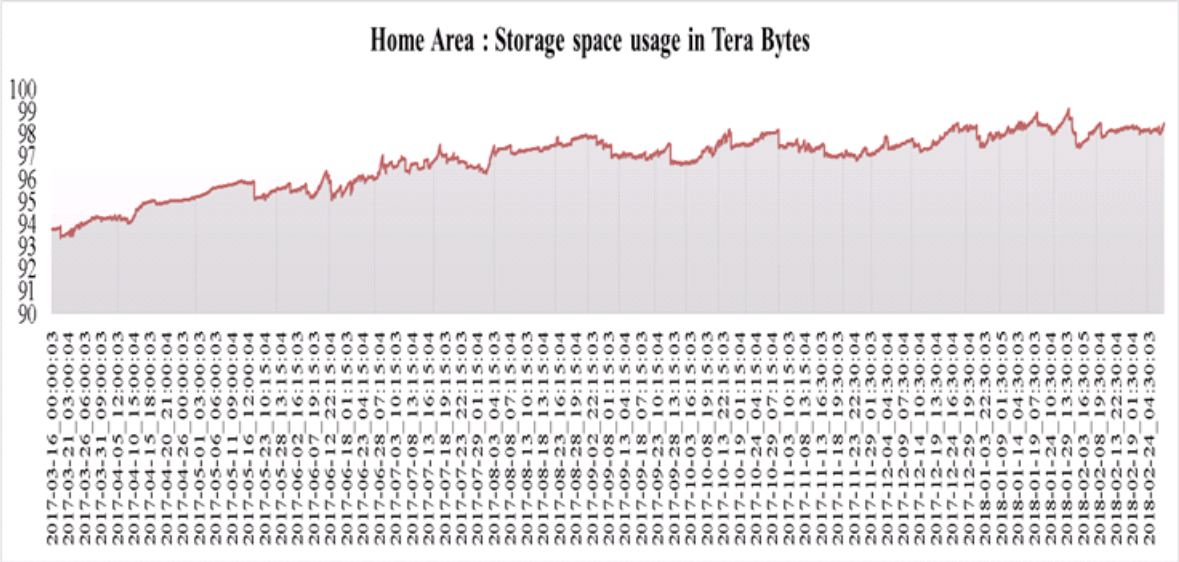
Table: Distribution of job wait time w.r.t. queues

| | Job waittime in Hours | |
|---|---|---|
| Queue | 2016-17 | 2017-18 |
| BIGJOBq | 75387.96611 | 450482.0942 |
| BURSTq | 1701836.04 | 97860.94333 |
| DDRq | 122.1055556 | 548202.7439 |
| FDRq | 150904.5736 | 11.82888889 |
| GPUq | 4496.0275 | 19122.91639 |
| SDSq | 144643.11 | 352.0522222 |
| TESTq | 75387.96611 | 83236.03667 |

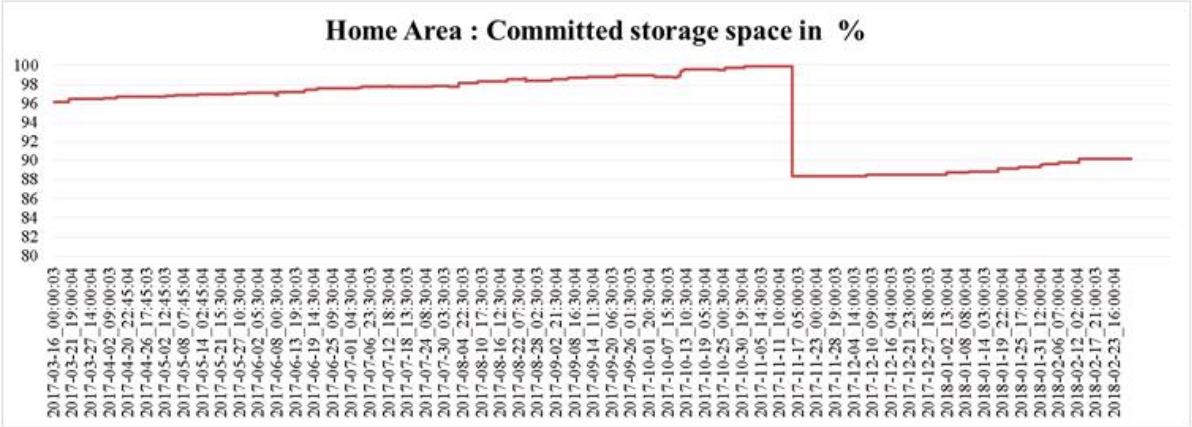
## 4.4 Storage

A HPC system is always coupled with one or more disk storage systems. Given the performance expected from such storage systems, they are distributed in nature, employing several I/O servers for increased throughput. At NPSF, two such storage systems are commissioned 1) Home Area, & 2) Scratch Area. Both of these said storage area are layered with POSIX compliant distributed and parallel filesystems respectively, with storage delivery over high-bandwidth, low-latency InfiniBand network. A third tape based storage system is used for scheduled backup of Home Area to mitigate data loss in event of failure.

Occupancy on both 1 and 2 is governed under policies for fair usage. Scratch Area is only available during job execution and for Home Area, every user has quota allocation with default being 100GB. The statistics of the Home Area are measured in terms of 1) total occupancy in respect to size and number of files 2) committed by way of on demand quota allocation as percentage of total available, and 3) percentage change at intervals in occupancy and number of files.

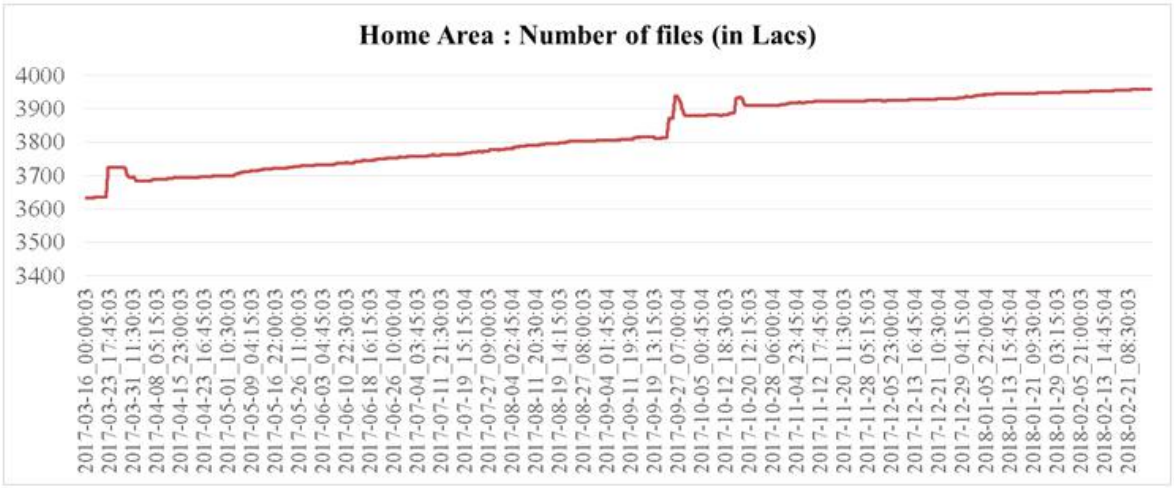



Above line plot depicts variations in total occupancy of Home Area. Total available size is 197 TB.



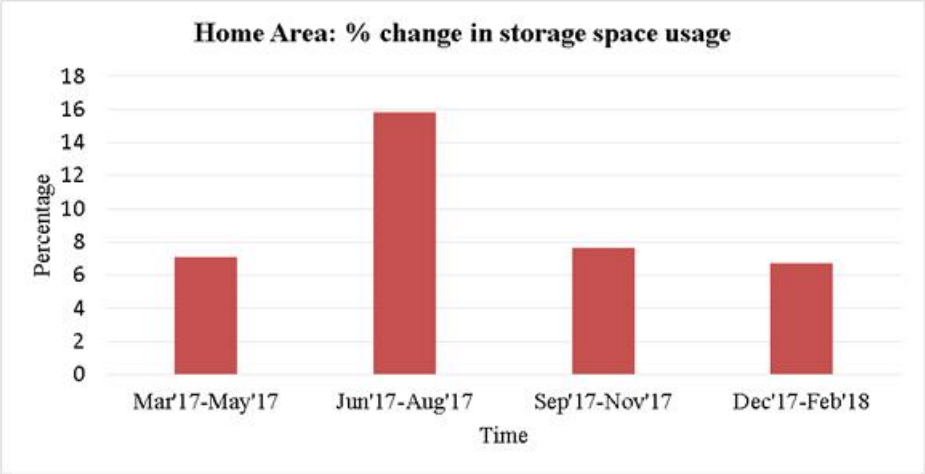

Above line plot presents total quota allocations during last year as percentage of total capacity. Notable dip 12% was due to reclamation exercise carried out by NPSF as quota allocations made neared 100%.

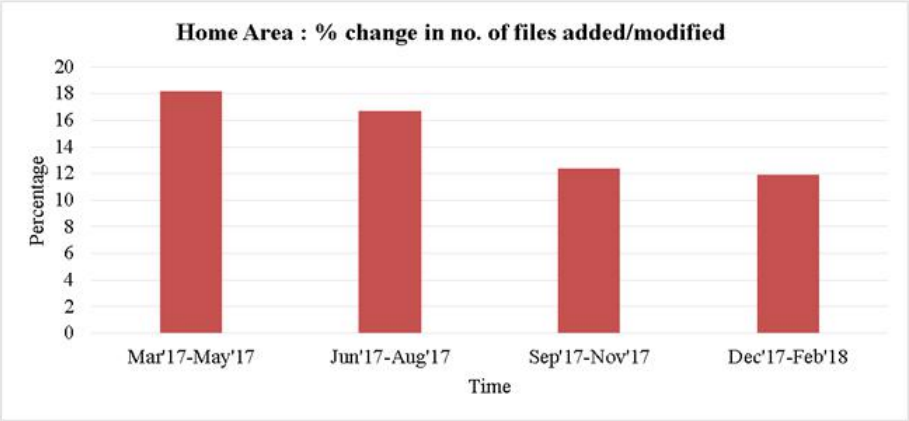
This can be seen as an indicator for the requirement of expansion of the storage.




Above line plot depicts variations in occupancy of Home Area in terms of number of files.

The below statistics shows % change in data size and % change in number of files which defines the need of backing up the data at regular intervals with incremental backup. If the % change in data/ no. of files becomes equal to the actual occupied storage, then the backup policy should be changed from incremental to full dump. The above statistics shows that we can continue with the incremental backup sessions.


Home Area: % change in storage space usage
Percentage
18
16
14
12
10
8
6
4
2
0
Mar'17-May'17
Jun'17-Aug'17
Sep'17-Nov'17
Dec'17-Feb'18
Time


Home Area : % change in no. of files added/modified
Percentage
20
18
16
14
12
10
8
6
4
2
0
Mar'17-May'17
Jun'17-Aug'17
Sep'17-Nov'17
Dec'17-Feb'18
Time

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# 5

# Publication Reports and Work Reports

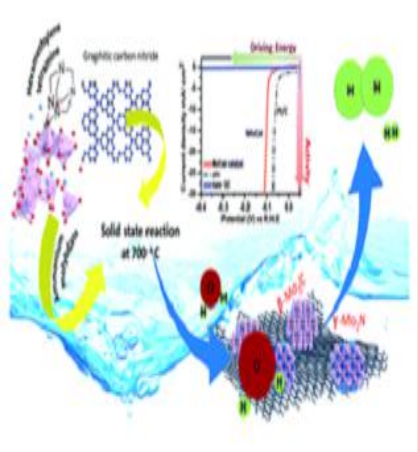
Some of the publication reports and work reports based on the research publication/s in high impact journals and the work that has been carried out on NPSF.

**Energy conversion/harvesting in 2D materials, Nanocatalysis**

**CI:** Dr. Abir De Sarkar, abir@inst.ac.in, abirdesarkar@gmail.com

**INSTITUTION:** INST Mohali

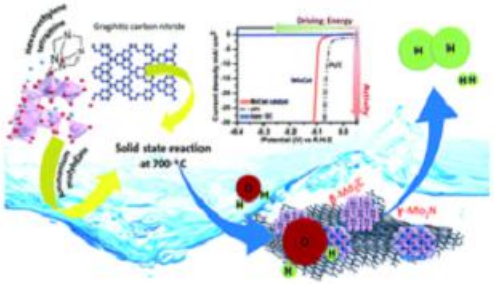
**RESEARCH DOMAIN:** Nanomaterials for clean, renewable and alternative energies, and clean environment




**Research Challenge:** Density functional theory based calculations are highly computationally intensive and demanding. Therefore, the challenge lies in studying large systems and running some calculations for a long duration of time (say, more than 72 hrs)

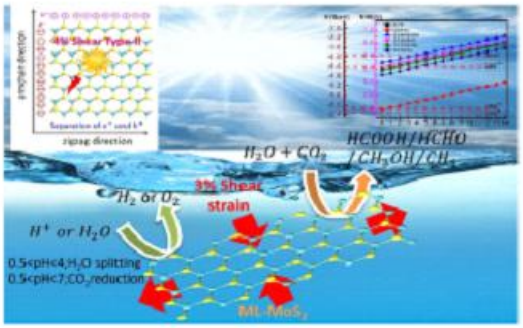
**Approach:** Density functional theory based methods

**Results (Graphs etc.):**



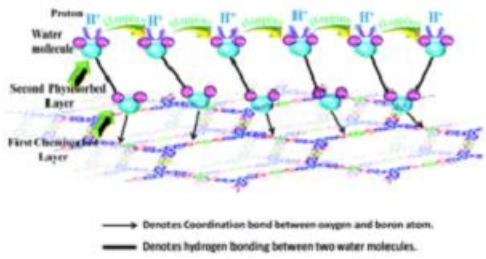
Nano-structured hybrid molybdenum carbides/nitrides generated *in situ* for hydrogen evolution reaction

*J. Mater. Chem. A*, 2017, **5**, 7764-7768



Strain and pH facilitated artificial photosynthesis in monolayer $MoS_2$ nanosheets

*J. Mater. Chem. A*, 2017, **5**, 22265-22276



A porous, crystalline truxene-based covalent organic framework and its application in humidity sensing

*J. Mater. Chem. A*, 2017,**5**, 21820-21827

**Impact:** Our computational findings have significantly advanced the current understanding on energy conversion/harvesting in 2D Materials. Our results provide very useful pointers and guidance to experimentalists and technologists. Besides our independent pursuit of research projects, we provide strong theoretical support to experimentalists.

Synergistic effects have been found in combining molybdenum carbide with molybdenum nitride nanoparticles, if synthesized in situ via a controlled solid-state reaction; thereby leading to an excellent hydrogen evolution reaction (HER) activity. Theoretical studies corroborate the experimental findings. An appreciable charge transfer at the interface of Mo2C and Mo2N nanoparticles facilitate the HER. This is further substantiated by the calculations of Gibbs free energy, which reaches very close to that of the commercially available Pt/C catalyst.

Photoconversion of carbon dioxide with water into renewable solar fuels using a single integrated system is the primary goal of artificial photosynthesis. The ease of applying mechanical strain reversibly in low dimensional materials can be exploited in optimizing their artificial photosynthetic or photocatalytic properties. Strain effects on the concerted interplay of all the factors controlling the photocatalytic ability have been comprehensively studied on monolayer MoS2nanosheets and calibrated, using density functional theory, to ascertain the type and magnitude of strain under which the artificial photosynthetic properties are optimally utilizable. Additionally, the role of pH has been carefully addressed.

The first example has been demonstrated in which truxene has been used as a building block to successfully synthesize novel covalent organic frameworks (COFs). DFT calculations have shown a good agreement between the experimental and simulated powder X-ray diffraction (PXRD) patterns and pore size distribution of this framework. COFs have shown great potential in emerging sensing applications.

I have been invited to present my research groups work at National and International Conferences. Our paper published in Journal of Physics: Condensed Matter 29 (2017) 225501 (7pp) has been selected for the 2017 Journal highlights. My Ph.D. students have presented their work in the form of Poster in Conferences.

**How this research work is benefited using NPSF:**

PARAM Yuva II has helped me immensely in guiding my Ph.D. students and Postdoc on these research problems. Without the strong support of PARAM Yuva II, coming up with such good Publications would not have been possible.

**Experiences using NPSF(system, support etc.):**

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. We have mainly been using VASP software.

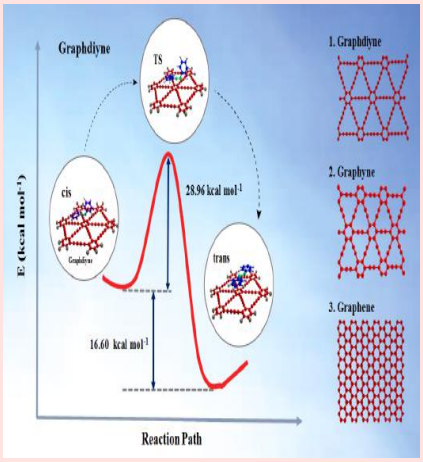
**Any other information:** CDAC, Pune has been doing a wonderful job for many years in helping Computational Scientists in their active pursuit of research, across India. The strong computational support provided by CDAC-Pune enables us to pursue good quality research. I would like to appeal to the Govt. 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, as it 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.

## Molecular Switching on Graphyne and Graphdiyne: Realizing Functional Carbon Networks in Synergy with Graphene

**CI:** Dr. R. S. Swathi swathi@iisertvm.ac.in

**INSTITUTION:** IISER Trivandrum

**RESEARCH DOMAIN:** Solar thermal fuels and data storage devices

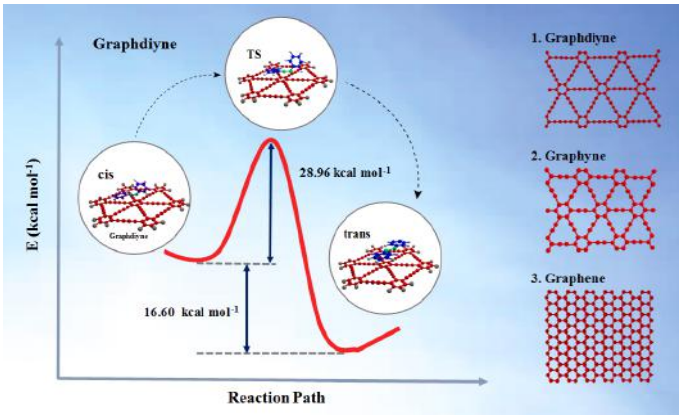



**Research Challenge:** Photoisomerization of molecules directly adsorbed on substrates is found to be either suppressed or enhanced depending upon the type of the substrate. A major goal, relevant to the development of future applications, is therefore to understand and control structural changes of molecular switches such as azobenzene (AZO) and its derivatives when adsorbed on suitable substrates.3. Photoisomerization of molecules directly adsorbed on substrates is found to be either suppressed or enhanced depending upon the type of the substrate. A major goal, relevant to the development of future applications, is therefore to understand and control structural changes of molecular switches such as azobenzene (AZO) and its derivatives when adsorbed on suitable substrates.3. Photoisomerization of molecules directly adsorbed on substrates is found to be either suppressed or enhanced depending upon the type of the substrate. A major goal, relevant to the development of future applications, is therefore to understand and control structural changes of molecular switches such as azobenzene (AZO) and its derivatives when adsorbed on suitable substrates.

exact underlying physical mechanism has remained elusive so far. toisomerization of molecules directly adsorbed on substrates is found to be either suppressed or enhanced depending upon the type of the substrate. A major goal, relevant to the development of future applications, is therefore to understand and control structural changes of molecular switches such as azobenzene (AZO) and its derivatives when adsorbed on suitable substrates.

**Approach:** Employing electronic structure calculations, we probe structures, energetics, kinetics and reaction pathways of thermal cis-trans isomerization of AZO and disperse orange 3 (DO3) adsorbed on the surfaces of graphyne (GY) and graphdiyne (GDY), newbies in the family of two-dimensional carbon networks and compared our results with those of graphene.

**Results:** Initially, we considered the adsorption of cis- and trans- forms of AZO and DO3 on the carbon networks. Our studies reveal that the trans isomers form most stable complexes due to - stacking. Additionally, the presence of substituent groups in DO3 contributes to the formation of more stable complexes than in case of AZO. The computed adsorption energies of molecular switches on the carbon networks lie between the range of physisorption and chemisorption energies, suggesting that the carbon networks can be excellent substrates on which the switches can undergo facile isomerization. Therefore, we investigated the thermodynamics, kinetics and reaction pathways of the isomerization process on the carbon networks and compared the results with those obtained for isolated molecular switches. The minimal change in the computed 5. activation barriers and high thermal storage capacity on adsorption indicate that GY and GDY could be used as substrates in conjunction with graphene in real devices.




**Impact:** The current work represents the first attempt, theoretical or experimental, in probing molecular switching on GY and GDY, which can have potential impact in the areas of solar thermal fuels and data storage devices. We also believe that our study motivates further theoretical and experimental studies to probe isomerization involving various other derivatives of AZO. Ultimate objective of such studies is to guide in the realization of various photoswitching molecules for real devices.

**How this research work is benefited using NPSF:**

The carbon networks (graphene, GY and GDY) studied in the current work are represented by cluster-based model systems. However, to study the effect of the size of the model systems representing the carbon networks, we need to consider larger cluster models, which are computationally very demanding. With the help of PARAM Yuva II, we were able to consider the molecules such as $C_{54}H_{18}$, $C_{66}H_{18}$ and $C_{90}H_{18}$ as representatives for graphene, GY and GDY, respectively and could calculate the energetics, thermodynamics and kinetics. Our study on photoswitching of two diverse azo-based systems, AZO and DO3 on carbon nanostructures is an interesting step forward along these lines. In our studies, for the first time, we obtained the TSs for the cis-trans isomerization of AZO and DO3 on the surfaces of GY and GDY. Such an analysis has not been so far carried out, even on graphene surface and would not have been possible without the excellent resources from PARAM Yuva II. Thus, using the facility, our computations demonstrated that GY and GDY can render excellent platforms for the isomerization of azo-based compounds.

**Experiences using NPSF(system, support etc.)**

PARAM Yuva II provided us easy access, less waiting time to run the jobs, and good technical support.

**Title of the work carried out:** Energy conversion in single layer MoS2

**Name & Designation of the Chief Investigator:** Dr. Abir De Sarkar, Scientist-E/Assoc. Prof.

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

**Institution Name:** Institute of Nano Science and Technology (Department of Science and Technology, Government of India), Phase - 10, Sector - 64 , Mohali, Punjab-160 062

**Research Challenge/s:** Studying large systems, which can be highly computationally intensive and demanding & also running some calculations for a long duration of time (say, more than 72 hrs)

**Work carried / Milestone / Achievements:** Presented Invited talks, Published papers, Our paper published in the Journal of Physics: Condensed Matter 29 (2017) 225501 (7pp) has been selected for the 2017 Journal highlights, Students have presented posters in Conferences

**Publications / Articles etc. (If any):**

1. Dimple, Nityasagar Jena, AshimaRawat, Abir De Sarkar*, "Strain and pH facilitated artificial photosynthesis in monolayer MoS2nanosheet", Journal of Materials Chemistry A, 5 (2017) 22265-22276

2. Harpreet Singh, Vijay K. Tomer, Nityasagar Jena, InduBala, Nidhi Sharma, DevadduttaNepak, Abir De Sarkar*, KamalakannanKailasam*, Santanu Pal*, "Truxene based Porous, Crystalline Covalent Organic Frameworks and its Applications in Humidity Sensing", Journal of Materials Chemistry A, 5 (2017) 21820-21827

3. Nityasagar Jena, Dimple, ShounakDhananjayBehere, Abir De Sarkar*, "Strain Induced Optimization of Nanoelectromechanical Energy Harvesting and NanopiezotronicResponse in MoS2 Monolayer Nanosheet", Journal of Physical Chemistry C 121 (2017) 91819190

4. Dimple, Nityasagar Jena, Abir De Sarkar*, "Compressive strain induced enhancement in thermoelectric-power-factor in monolayer MoS2nanosheet", Journal of Physics: Condensed Matter 29 (2017) 225501 (7pp) (Selected for 2017 Journal highlights)

5. Rajinder Kumar, Ritu Rai, Seema Gautam, Abir De Sarkar, N. Tiwari, Shambhu Nath Jha, Dibyendu Bhattacharyya, Ashok K Ganguli and VivekBagchi, Nano-structured hybrid Molybdenum Carbides/Nitrides generated in-situ for HER Applications, Journal of Materials Chemistry A 5 (2017) 7764-7768

6. Neha Wadehra, RuchiTomar, SoumyadipHalder, Minaxi Sharma, Inderjit Singh, Nityasagar Jena, Bhanu Prakash, Abir De Sarkar, ChandanBera, AnanthVenkatesan, S Chakraverty, "Electronic structure modification of the KTaO3 single-crystal surface by Ar+ bombardment", Physical Review B, 96 (2017) 115423

**Appreciation / Recognition (if any):** Have been invited to present my work at both National and International levels

**Benefits & experience of using NPSF:**

PARAM Yuva II has helped me immensely in guiding my Ph.D. students and my Postdoc 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.

**Any other relevant information (if any):** 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 ParamYuva II is really high. ParamYuva 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.

**Title of the work carried out:** Spin-induced transition metal (TM) doped SnO2 a dilute magnetic semiconductor (DMS): A first principles study

**Name & Designation of the Chief Investigator:** Dibya Prakash Rai (D. P. Rai)

**E-mail Id:** dibyaprakashrai@gmail.com

**Institution Name:** Pachhunga University College, Aizawl Mizoram India.

**Work carried / Milestone/Achievements:** is submitted to Journal of Physics and Chemistry of Solids, Elsevier (Under Review)

**Publications / Articles etc. (If any):** This work is submitted to Journal of Physics and Chemistry of Solids, Elsevier (Under Review)

**Awards (If any):** Received outstanding Reviewer award for 2017 from Material Research Express (IOP).

**Appreciation / Recognition (if any):** Received outstanding Reviewer award for 2017 from Material Research Express (IOP).

**Benefits & experience of using NPSF:**

It is beneficial. But I dont know why most of the time when I submit the job it goes in queue. It takes long time to complete the job. Please kindly look into the matter.

**Title of the work carried out:** Molecular Simulation Study of the Phase Behaviour of Complex Compounds in Advanced Biofuels

**Name & Designation of the Chief Investigator:** Jhumpa Adhikari, Professor

**E-mail Id:** adhikari@che.iitb.ac.in

**Institution Name:** IIT Bombay

**Research Challenge/s:** Predict phase behavior of oxygen-containing compounds present in biofuels, such as glycerol, levulinic acid and their mixtures using molecular simulation techniques.

**Work carried / Milestone/Achievements:** Extended GC-TMMC code for mixtures of simple model fluids to investigate behavior of complex molecules

**Publications / Articles etc. (If any):** Phase Equilibria and Critical Point Predictions of Mixtures of Molecular Fluids Using Grand Canonical Transition Matrix Monte Carlo TamaghnaChakraborti and JhumpaAdhikari Industrial & Engineering Chemistry Research 2017 56 (22), 6520-6534 DOI: 10.1021/acs.iecr.7b01114

**Benefits & experience of using NPSF:**

The cluster is well-maintained and has UPS facilities which allow us uninterrupted use of computational facilities. We are grateful for the facilities made available to us.

**Title of the work carried out:**

1. Theoretical Study of the Decomposition Pathways of Perbenzoate anion.
2. Unimolecular decomposition of formamide via direct chemical dynamics simulations

**Name & Designation of the Chief Investigator:** Dr. Manikandan Paranjothy, Assistant Professor

**E-mail Id:** pmanikandan@iitj.ac.in

**Institution Name:** Indian Institute of Technology Jodhpur

**Research Challenge/s:** The technology we use in our research group is called Direct Dynamics Simulations which we employ to study organic reaction mechanisms, decomposition pathways, branching ratios, etc, for interesting chemical and biochemical reactions. This technique requires integration of Newtons equations and the required potentials and forces for the integration are computed on-the-fly using a chosen level of electronic structure theory (quantum chemistry). In general, one requires to generate atleast 100 classical trajectories in a simulation. Assuming integration to be carried out till 3 picosecond (3000 femtosecond) and an integration stepsize of 1 femtosecond, we need to perform 3000 single point electronic structure calculations for one trajectory. For 100 trajectories, we need to perform 3000*100 = 300000 single point electronic structure calculations. Please note that the values reported here are bare minimum requirements for classical trajectory simulations and only with increase in number of trajectories, the accuracy of the results improve. To carry out such an enormous amount of calculations, we utilized the CDAC PARAMYuva II facility.

**Work carried / Milestone/Achievements:** Between the period 16/03/2017 to 28/02/2018, we computed direct dynamics trajectories for two systems (1) Perbenzoate anion which contains 15 atoms (71 electrons) and (2) formamide which contains 6 atoms (24 electrons). We generated 40 (out of 100 total) trajectories and 150 (out of total 300) trajectories using the PARAM Yuva II facility during the mentioned period. These calculations were carried out using the B3LYP functional with a medium sized basis set. Without the PARAM Yuva II facility, it is possible that these calculations would have taken much longer periods of time with the small facility we have in IIT Jodhpur.

**Publications / Articles etc.** We have published two nice papers in high quality research journals reporting the results partially generated using the PARAN yuva II facility.

1. Y. Krishnan, P. Rajbhangshi, and M. Paranjothy, Theoretical study of perbenzoate anion decomposition pathways in the gas phase, Int. J. Mass Spectrom. 428, 8 (2018).
2. A. Gaulaut and M. Paranjothy, Unimolecular decomposition of formamide via direct chemical dynamics simulations, Phys. Chem. Chem. Phys. (In press).

**References:**

**Benefits & experience of using NPSF:**

As mentioned above, our simulations are memory and processor intensive which we could smoothly carry out in the PARAM Yuva II facility. Many different compilers are available in the facility and we could select the right compiler for our codes. We definitely look forward to using the facility continuously.

**Title of the work carried out:** To study the properties of doping of Al, Cu and Mn in ZnO thin films using DFT and to study of magnetic properties of Ising thin films using Computer Simulation

**Name & Designation of the Chief Investigator:** Dr. Pradip Bhausaheb Shelke, Head and Associate Professor, Department of Physics, Ahmednagar College Ahmednagar

**E-mail Id:** shelke.pradip@gmail.com

**Institution Name:** Department of Physics, Ahmednagar College Ahmednagar

**Research Challenge/s:** Our area of research is Material Simulation using Density Functional Theory (DFT) and Monte Carlo simulation methods. This work is a intense work requiring a good computational facility with parallel environment. Presently, we do not have such facility in our institute. However, due to invaluable help of CDAC we are able to overcome this challenge.

**Work carried / Milestone/Achievements:** Using computational facility of CDAC we have carried out following work. We have studied the graphatic phase formation in few layer ultrathin ZnO thin films using DFT. Also, we have studied effects of doping of elements like Al, Cu, and Mn in graphitic thin films. Now, we are analyzing the data and preparing manuscript. Also, we have studied magnetic properties of Ising thin films using Computer Simulation.

**Publications / Articles etc. (If any):**

1. Magnetic properties of patterned thin ising films, communicated to Journal of Modern Physics B (world Scientific Publishers, Singapore)
2. Dynamics of Random Sequential Adsorption (RSA) of linear chains consisting of n circular discs - Role of aspect ratio and departure from convexity, Pradip B. Shelke, A.V. Limaye, Surface Science 637638 (2015) 14.
3. Random sequential adsorption of coupled three-circle objects for various radius ratios, Pradip B. Shelke and A. V. Limaye , Physical Review E 83, 061607 (2011).
4. Blocking effects in irreversible adsorption of linear macromolecules,Pradip B. Shelke, A.G. Banpurka, S.B. Ogale, A.V. Limaye, Surface Science 601 (2007) 274279.
5. Simulation studies of Cooperative Sequential Adsorption (CSA) of binary mixture, Pradip B. Shelke, NCANAP2013 PROCEEDING (Feb.2013) 149 - 150

**Awards (If any):** Received Bhaskar Raye award for best senior college Physics teacher from Indian Physics Association Pune Chapter on 4th September 2017 at Department of Physics, Savitribai Phule Pune University.

**References:** Dr. A. V. Limaye, Department of Physics, Savitribai Phule Pune University

**Benefits & experience of using NPSF:**

PARAM Yuva II facility is really beneficial for us. Especially, we like the facility of submitting test run without queue.

**Any other relevant information (if any):** Under my guidance two students are working for their Ph.D. and two students for their M.Phil. degrees.

**Title of the work carried out:** Quantum transport in elemental doped 2D monolayer and atomic clusters

**Name & Designation of the Chief Investigator:** Dr Sanjeev Kumar Gupta Assistant Professor

**E-mail Id:** sanjeev.gupta@sxca.edu.in

**Institution Name:** St. Xaviers College, Ahmedabad, Gujarat

**Research Challenge/s:** Our cost-effective and less time consuming strategy proposed in this work will assist in improving the realistic functional design of photovoltaic materials in the laboratory towards the next stage.

**Work carried / Milestone/Achievements:**
During the time period from 16th March, 2017 to 28th February, 2018, we have completed three major projects.

1. First, we have systematically investigated the electronic and optical properties of single-layer arsenene with two types of functionalized organic molecules; an electrophilic molecule [tetracyanoquinodimethane (TCNQ)] and a nucleophilic molecule [tetrathiafulvalene (TTF)], as an electron acceptor and electron donor, respectively.The interfacial charge transfer between the arsenene monolayer and TCNQ/TTF molecules extensively reduces the band gap of arsenene and accordingly resulted in a p- or n-type semiconducting behavior, respectively. We have also performed the interfacial charge transfer from organic molecules to monolayer arsenene and vice versa. The interfacial surface molecular modification has established an efficient way to develop the light harvesting of arsenene in different polarization directions. Our theoretical investigation suggests that such n- and p-type arsenene semiconductors would broaden the applications in the field of nanoelectronic and optoelectronic devices such as photodiodes and it is also useful for constructing functional electronic systems.

2. Secondly, we have presented a thorough study of electronic and optical properties and interface charge dynamics,that revealed CaMnO3as a better candidate for the electron transport material in thin film hole transporting material free hybrid perovskite solar cells with the planar architecture than the most common anatase TiO2.The interfacial charge transfer between the arsenene monolayer and TCNQ/TTF molecules extensively reduces the band gap of arsenene and accordingly resulted in a p- or n-type semiconducting behavior, respectively. We have also performed the interfacial charge transfer from organic molecules to monolayer arsenene and vice versa. The interfacial surface molecular modification has established an efficient way to develop the light harvesting of arsenene in different polarization directions. Our theoretical investigation suggests that such n- and p-type arsenene semiconductors would broaden the applications in the field of nanoelectronic and optoelectronic devices such as photodiodes and it is also useful for constructing functional electronic systems.

3. And recently, we have studied the structural, electronic and optical properties of single-layer carbon phosphide (CP) allotropes (a-, b- and c-phases) based on density functional theory. The thermoelectric properties like electrical conductivity, thermal conductivity, thermoelectric power, figure of merit (ZT) and compatibility factor as a function of temperature are calculated by using BoltzTrap code. The electronic band structures reveal the direct band gap of a- and b-CP monolayer (i.e., semiconducting nature), while c-CP monolayer is

semimetallic with Dirac fermions. The significant absorption is observed in a-, b- and c-CP monolayer, which can be used as an ultraviolet opticalnanodevice, and all three phases of monolayer of CP are directionally transparent. The transmission spectrum of monolayer of b- and c-phase in the visible region is much higher; therefore, it is used in an anti-reflecting layer in solar cell also. The a-phase of CP monolayer in the ZT increases linearly up to 1500 K, and beyond it reached maximum values as compared to other phases. The results show that below 550 K, CP allotropes (both n- and p-types) are hitherto the best-promising thermoelectric materials. These theoretical investigations suggest that the different phases of semiconducting materials of CP are better candidate for potential application in micro-/nanoscale device, photovoltaic and optoelectronics.

**Publications / Articles etc. (If any):**


1. Singh, D., Kansara, S., Gupta, S.K. and Sonvane, Y., Single layer of carbon phosphide as an efficient material for optoelectronic devices. Journal of Materials Science, pp.1-14.

2. Pandey, K., Singh, D., Gupta, S.K., Yadav, P., Sonvane, Y., Lukaevi, I., Kumar, M., Kumar, M. and Ahuja, R., 2018. Improving electron transport in the hybrid perovskite solar cells using CaMnO3-based buffer layer. Nano Energy.

3. Singh, D., Gupta, S.K., Sonvane, Y. and Sahoo, S., 2017. Modulating the electronic and optical properties of monolayer arsenene phases by organic molecular doping. Nanotechnology, 28(49), p.495202.


**Appreciation / Recognition (if any):** Received award and citation "Researcher of the year 2017", for the outstanding contribution in the field of physics, St. Xavier's College, Ahmedabad, Gujarat

**References:**


1. Singh, D., Kansara, S., Gupta, S.K. and Sonvane, Y., Single layer of carbon phosphide as an efficient material for optoelectronic devices.Journal of Materials Science, pp.1-14.

2. Pandey, K., Singh, D., Gupta, S.K., Yadav, P., Sonvane, Y., Lukaevi, I., Kumar, M., Kumar, M. and Ahuja, R., 2018.Improving electron transport in the hybrid perovskite solar cells using CaMnO 3-based buffer layer. Nano Energy.

3. Singh, D., Gupta, S.K., Sonvane, Y. and Sahoo, S., 2017. Modulating the electronic and optical properties of monolayer arsenene phases by organic molecular doping.Nanotechnology, 28(49), p.495202.


**Benefits & experience of using NPSF:**

The proposed work is one of the important directions both in the fundamental and applied sciences. In addition, the outcome will be beneficial for the research students participating in the projects giving them opportunity to perform scientific investigation at national/international level and to meet and discuss with scientist and students from other international laboratory. This supercomputing collaboration can also be extended for the future.It is expected that the studies performed will lead to publications in refereed international journals and will be suitable for presentation at local and international conferences.

**Any other relevant information (if any):**

J Mater Sci
Electronic materials

# Single layer of carbon phosphide as an efficient material for optoelectronic devices

Deobrat Singh[1], Shivam Kansara[1], Sanjeev K. Gupta[2,*], and Yogesh Sonvane[1,*]

[1] Advanced Materials Lab, Department of Applied Physics, S.V. National Institute of Technology, Surat 395007, India
[2] Computational Materials and Nanoscience Group, Department of Physics, St. Xavier's College, Ahmedabad 380009, India

## Acknowledgements

Helpful discussions with Prof. Ravindra Pandey, Dr. Gaoxue Wang and Mr. Kaptan Rajput are gratefully acknowledged. SKG also acknowledges the use of high-performance computing clusters at IUAC, New Delhi, and YUVA, PARAM II, Pune, to obtain the partial results presented in this paper. SKG also

Nano Energy 45 (2018) 287–297

Contents lists available at ScienceDirect

Nano Energy

journal homepage: www.elsevier.com/locate/nanoen

Full paper

# Improving electron transport in the hybrid perovskite solar cells using $CaMnO_3$-based buffer layer

Kavita Pandey[a], Deobrat Singh[b], S.K. Gupta[c,*], Pankaj Yadav[a,*], Yogesh Sonvane[b], Igor Lukačević[d,*], Manjeet Kumar[e], Manoj Kumar[a], Rajeev Ahuja[f]

## Acknowledgements

Authors I.L. and S.K.G. acknowledge the financial support from the "Gost istraživač" project (INGI-2015-7). S.K.G. acknowledges the usage of high performance computing clusters: (a) K2-IUAC, New Delhi, India, (b) YUVA, PARAM-II, Pune, India to obtain the partial results presented

IOP Publishing Nanotechnology
Nanotechnology 28 (2017) 495202 (11pp) https://doi.org/10.1088/1361-6528/aa9430

# Modulating the electronic and optical properties of monolayer arsenene phases by organic molecular doping

Deobrat Singh[1], Sanjeev K Gupta[2,4], Yogesh Sonvane[1,4] and Satyaprakash Sahoo[3]

## Acknowledgments

S K G and Y A S thank the Science and Engineering Research Board (SERB), India, for the financial support (Grant nos. YSS/2015/001269 and EEQ/2016/000217, respectively). S K G also acknowledges the use of high performance computing clusters at IUAC, New Delhi and YUVA, PARAM II, Pune to obtain the partial results presented in this paper. D S would like to thank the University Grant Commission (UGC), New Delhi, India, for the financial support.

**Title of the work carried out:** Density functional theory/time dependent density functional theory (DFT/TDDFT) study of boron clusters.

**Name & Designation of the Chief Investigator:** Dr. Siddheshwar Chopra, Assistant Professor

**E-mail Id:** sidhusai@gmail.com

**Institution Name:** Amity University

**Research Challenge/s:** DFT/ TDDFT calculations which need high computational resources.

**Work carried / Milestone/Achievements:** Optical properties were determined using DFT,TDDFT calculations.

**Benefits & experience of using NPSF:**

I have been using this facility for 3 years or so, and I can undoubtedly rate it the best facility due to its computational power and most importantly the superb support team where people are always ready to assist you in case of any difficulty. I never faced any problems ever.

**Title of the work carried out:**

1. Fluctuation dynamo action in compressible turbulence (by Sharanya Sur)
2. Heating of the solar atmosphere (by Piyali Chatterjee)

**Name & Designation of the Chief Investigator:** Sharanya Sur, Reader

**E-mail Id:** sharanya.sur@iiap.res.in, piyali.chatterjee@iiap.res.in

**Institution Name:** Indian Institute of Astrophysics

**Research Challenge/s:**

1. Shocks and contact discontinuities are two basic kinds of noncontinuous features encountered in astrophysical flows. Treatment of shocks in compressible turbulent flows are challenging as they involve discontinuous changes in the density, pressure, temperature and velocities. Unless preventive measures are taken, shocks can trigger self-amplifying instabilities which can kill the simulation. In our work, we have simulated fluctuation dynamos in high Mach number turbulent flows (as occurs in galaxies) with the help of Riemann solvers in the publicly available FLASH code.
2. Short time steps ( 0.1 ms) due to field aligned Spitzer conductivity and time step constraints due to numerical solution of detailed radiative transfer equation at low opacity using long characteristics method. Grid size of 25 km required near the transition region of the sun where the temperature rises steeply from 8000 K to 40000K.

**Work carried / Milestone/Achievements:**

- Fluctuation dynamo action in compressible turbulence
    1. Simulating fluctuation dynamos in high Mach number turbulent flows.
    2. Probing the degree of coherence of the generated field and the Faraday rotation measure (RM) obtained from such fields.
    3. Extent to which the computed RM compares with observational estimates from MgII absorption systems.
- Heating of the solar atmosphere
    1. Development of a 3-dimensional realistic solar atmosphere using the pencil code.
    2. Non uniform grid and radiative transfer.
    3. Non local mean field stellar dynamos

**Publications / Articles etc. (If any):**

1. Strong nonlocality variations in a spherical mean-field dynamo, Brandenburg A. Chatterjee, P. 2018, to appear in AstronNachr (eprint arXiv:1802.04231)

2. Applying the weighted horizontal magnetic gradient method to a simulated flaring Active Region, Korsos, M., Chatterjee, P. & Erdelyi, R. 2018 (under review/revision in ApJ)

3. Faraday rotation signatures of fluctuation dynamos in young galaxies, Sharanya Sur, Pallavi Bhat & Kandaswamy Subramanian, 2018, MNRAS Letters, 475, L72 - L76 (eprint arXiv:1711.08865).

**Any other relevant information (if any):**

1. Quick availability of a debugging queue using about 128 cores for at least 2 hours without having to wait too long in the queue will be of great help.

2. Long waiting time in the queue (usually 14 days, sometimes up to 21 days) when running jobs using more than 512 cores. This implies, that only 1-2 such high resolution simulations can be performed in a month. It will be beneficial if the wall clock time limit in the BURSTq mode is increased to at least 72 hrs from the current limit of 17:55.

3. Segregate jobs which use less than 1 - 128 cores to run on a separate machine and reserve 2500 cores for running jobs which require 512 - 2048 cores.

**Title of the work carried out:** Molecular Dynamics Analysis of Nanocomposites

**Name & Designation of the Chief Investigator:** Dr. Mohammed Rabius Sunny, Assistant Professor, Department of Aerospace Engineering, Indian Institute of Technology Kharagpur.

**E-mail Id:** sunny@aero.iitkgp.ernet.in

**Institution Name:** Indian Institute of Technology Kharagpur

**Research Challenge/s:** Nanocomposite models are in the scale of Nano-meters, its merely impossible to carry out the experimental study on Nano-level. We have chosen Molecular Dynamics as our soft-experiment tool to analyze the Nanocomposites. Molecular Dynamics study involves the interactions of each and every particle present in the system, so it leads high computational cost. Work carried / Milestone/Achievements: We have carried out our research study on the Nanocomposite comprises of Carbon Nanotube and Polymer matrix.

**References:**

1. Zhu, R., Pan, E., Roy, a. K. K., & a.K. Roy. (2007). Molecular dynamics study of the stressstrain behavior of carbon-nanotube reinforced Epon 862 composites. Materials Science and Engineering: A, 447(12), 5157.
2. Kim, B.-H., Lee, K.-R., Chung, Y.-C., & Gunn Lee, J. (2012). Effects of interfacial bonding in the Si-carbon nanotube nanocomposite: A molecular dynamics approach. Journal of Applied Physics, 112(4), 44312.
3. Adnan, A., Sun, C. T., & Mahfuz, H. (2007). A molecular dynamics simulation study to investigate the effect of filler size on elastic properties of polymer nanocomposites. Composites Science and Technology, 67(34), 348356.
4. Rahman, R. (2012). Molecular Dynamics Modeling and Characterization of Graphene/Polymer Nanocomposites, 120.
5. Rahman, R., & Haque, A. (2011). Molecular Dynamics Simulation of Cross-linked Graphene-Epoxy Nanocomposites, (Md), 34.
6. Yu, S., Yang, S., & Cho, M. (2009). Multi-scale modeling of cross-linked epoxy nanocomposites. Polymer, 50(3), 945952.
7. Arash, B., Wang, Q., & Varadan, V. K. (2014). Mechanical properties of carbon nanotube/polymer composites. Scientific Reports, 4, 6479.

**Benefits & experience of using NPSF:**

The PARAM Yuva II facility was very useful and robust. We didnt find any difficulty to access the facility. The maintenance of job queues was very comfortable. Also the helpdesk support was flawless.

**Title of the work carried out:**

1. Project: Spectral decomposition of seismic data and its application for gas hydrates exploration
2. Work: Development of parallel environment for performing Local time frequency transform (LTF) of 2D/3D seismic data.

**Name & Designation of the Chief Investigator:** Ms. Richa Rastogi, Joint Director

**E-mail Id:** richar@cdac.in

**Institution Name:** High Performance Computing  Scientific and Engineering Application Group (HPC-S&EA), C-DAC

**Work carried / Milestone/Achievements:** Aim of this activity was to carry out Local time frequency decomposition (LTFD) of seismic 2D and 3D data sets. This spectral decomposition methods gives time-frequency images of input data which are in time-space domain. ISO-frequency sections are calculated for each input data set which are used to analyze amplitude variations of seismic data. LTFD technique is a compute intensive method.

We have written a parallel application for LTFD (SeisLTFD) using distributed computing environment of PARAM YUVA II. The developed application uses sfltft an open source program from Madagascar package and Message Passing Interface (MPI) for input data distribution among nodes. OpenMP APIs are also used for taking advantage of shared memory environment within each nodes. MPI-IO is utilized for enabling parallel io in the program.

This application was used to analyze amplitude variation in ISO-frequency sections of real field seismic data from Krishna Godavari basin, Blake ridge region and Netherland offshore region.

**References:**

Liu, Y. and Fomel, S., 2013, Seismic data analysis using local time-frequency decomposition; Geophysical Prospecting, 61, 516525. doi:10.1111/j.1365-2478.2012.01062.x

**Benefits & experience of using NPSF:**

Performing a LTFD of seismic trace is a compute intensive task. For a 2D sparker data (consisting of approximately 2000 traces) collected in Krishna Godavari basin, India, estimated execution time on single processor was approximately 2.5 days. However actual execution time with parallel program was 130 min using 2 node with 16 OpenMP threads per node. Analysis of sixteen 2D sparker data from Krishna Godavari basin was performed using parallel program. This reduction of execution time helped in completion of the project within specified time frame.

**Any other relevant information (if any):** The parallel program will be provided under GNU General Public License.

# 6

# Ph.D Theses

Total number of Ph.D theses in Year 2017-18 : 03

1. **Atomistic simulations of nanostructure and dynamics of phosphoric acid-benzimidazole systens: A fuel cell initiative**
   Student: Ms. Minal Pednekar
   Supervisor: Dr. Arun Venkatnathan
   Institute: IISER Pune

2. **Effect of functionalization and defect engineering on the properties of hBN/Nanocomposite**
   Student: Mr. Rajesh Kumar
   Supervisor: Prof. Avinash Prashar
   Institute: IIT Roorkee

3. **Thesis Title : Investigation of structural dynamics and allosteric mechanism of SAMHD1 protein complex via Molecular Dynamics studies.**
   Student: Mr. Kajwal Kumar Patra
   Supervisor: Prof. Swati Bhattacharya
   Institute: IIT Guwahati

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# 7

# Publications

Total number of publications by NPSF users in Year 2017-18: 66

**Publications by NPSF users**

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

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

*Chemistry of Materials* (9.466)

Sachin Rondiya, Nitin Wadnerkar, Yogesh Jadhav, Sandesh Jadkar, Santosh Haram, and Mukul Kabir, Structural, Electronic, and Optical Properties of Cu2NiSnS4: A Combined Experimental and Theoretical Study toward Photovoltaic Applications, Chemistry of Materials 29, 3133 (2017)

*J. Phys. Chem. Lett* (9.353)

S. Das, A. Dey. G. Reddy and D.D. Sarma, Suppression of the coffee-ring effect and evaporation-drive disorder to order transition in colloidal droplets, J. Phys. Chem. Lett., **8**, 4704, 2017.

*Journal of Materials Chemistry A* (8.867)

Rajinder Kumar, Ritu Rai, Seema Gautam, Abir De Sarkar, N. Tiwari, Shambhu Nath Jha, Dibyendu Bhattacharyya, Ashok K Ganguli and Vivek Bagchi, Nano-structured hybrid Molybdenum Carbides/Nitrides generated in-situ for HER Applications, Journal of Materials Chemistry A, **5** (2017) 7764-7768

Harpreet Singh, Vijay K. Tomer, Nityasagar Jena, Indu Bala, Nidhi Sharma, Devadutta

Nepak, Abir De Sarkar, Kamalakannan Kailasam and Santanu Pal, Truxene based Porous, Crystalline Covalent Organic Frameworks and its Applications in Humidity Sensing, Journal of Materials Chemistry A,**5** (2017) 21820-21827

Dimple, Nityasagar Jena, Ashima Rawat and Abir De Sarkar, Strain and pH facilitated artificial photosynthesis in monolayer MoS2 nanosheet, Journal of Materials Chemistry A, **5** (2017) 22265-22276

*Physics Review Letters* (8.462)

G. J. Sreejith, Stephen Powell and Adam Nahum, Emergent SO (5) symmetry at the columnar ordering transition in the classical cubic dimer model. (Submitted)

*ACS Applied Materials & Interfaces* (7.504)

Mayanglambam Manolata Devi, Kuljeet Kaur, Ankita Gupta, Chandan Bera, Ashok Kumar Ganguli and Menaka Jha , Conversion of waste tin containers to highly efficient photocatalyst based on SnO2-Fe3O4 heterostructures, (Submitted) ACS Applied Materials & Interface

*Carbon* (6.337)

S Chandra Shekar, R. S. Swathi, Molecular switching on graphyne and graphdiyne: Realizing functional carbon networks in synergy with graphene. Carbon 2018, **126**, 489-499

*ApJ* (5.333)

Korsos, M., Chatterjee, P. and Erdelyi, R, Applying the weighted horizontal magnetic gradient method to a simulated flaring Active Region, 2018 (under review/revision in ApJ)

*Chem. Eur. J.* (5.317)

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*Journal of Physical Chemistry C* (4.536)

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*ChemElectroChem* (4.136)

P. K. Gangadharan, S. M. Unni, N. Kumar, P. Ghosh and S. Kurungot, Nitrogen-Doped Graphene with Three-Dimensional Architecture Assisted by Carbon Nitride Tetrapods as an Efficient Metal-Free Electrocatalyst for Hydrogen Evolution, ChemElectroChem., **4**, 2643 (2017)

*Journal of Biological Chemistry* (4.125)

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*Physical Review B* (3.718)

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*Int. J. Biol. Macromol* (3.671)

Narang, S. S.; Shuaib, S.; Goyal, B. Molecular insights into the inhibitory mechanism of rifamycin SV against 2microglobulin aggregation: A molecular dynamics simulation study. Int. J. Biol. Macromol. 2017, **102**, 10251034.

*Atmospheric Environment* (3.629)

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*J. Cell. Biochem* (3.446)

Narang, S. S.; Shuaib, S.; Goyal, D.; Goyal, B. Assessing the effect of D59P mutation in the DE loop region in amyloid aggregation propensity of 2microglobulin: A molecular dynamics simulation study. J. Cell. Biochem. 2018, 119, 782792.

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*Applied Physics Letters* (3.411)

Renu Rani, Dimple, Nityasagar Jena, Anirban Kundu, Abir De Sarkar and Kiran Shankar Hazra, Controlled formation of Nanostructures on MoS2 Layers by Focused Laser Irradiation, Applied Physics Letters **110** (2017) 083101

*Polymer* (3.364)

Rajesh Kumar, Avinash Parashar, Effect of geometrical defects and functionalization on the interfacial strength of h-BN / polyethylene based nanocomposite. Polymer 2018 (Under review)

*J.Phys. Chem. B* (3.177)

Bappa Ghosh and Srabanti Chaudhury, Influence of the Location of Attractive Polymer Pore Interactions on Translocation Dynamics, J. Phys. Chem. B, **122**,360-368 (2018)

Dey and G. Reddy, Toroidal condensates by semiflexible polymer chains: Insights into nucleation, growth and packing defects, J.Phys. Chem. B, **121**, 9291, 2017.

Sangkha Borah and Padma Kumar Padmanabhan, First Principle Molecular Dynamics Investigation of Waterborne As-V Species, J. Phys. Chem. B(Submitted)

*J.Chem. Phys* (2.965)

Deepashri Saraf, Ashok Kumar, Dilip Kanhere and Anjali Kshirsagar, Size dependent tunnel diode effects in gold tipped CdSe nanodumbbells, J.Chem. Phys., **146**, 054703 (2017).

G. Singh, A. Nandi, S. R. Gadre, T. Chiba, A. Fujii, J., A Combined Theoretical and Experimental Study of Phenol (Acetylene)n (n 7) Clusters, Chem. Phys. **146**, 154303, 2017

*Catalysis Today* (2.94)

L. George, S. Sappati, P. Ghosh and R. Nandini Devi, Sensitizing with short conjugated molecules: Multimodal anchoring on ZnO nanoparticles for enhanced electron transfer characteristics, stability and H2 evolution, Catalysis Today. DOI:10.1016/j.cattod.2017.09.052

*J. Phys. Chem. A* (2.847)

Datar, A.; Hazra, A. Pathways for Excited-State Nonradiative Decay of 5, 6 Dihydroxyindole, a Building Block of Eumelanin. J. Phys. Chem. A, 2017, **121**, 2790-2797

Y. Krishnan, N. Sharma, U. Lourderaj and M. Paranjothy, Classical Dynamics Simulations of Dissociation of Protonated Tryptophan in the Gas Phase, J. Phys. Chem. A, 2017, **121**, 4389 4396

Manae, M. A.; Hazra, A. "Interplay between Conjugation and Size-Driven Delocalization Leads to Characteristic Properties of Substituted Thymines." J. Phys. Chem. A, 2017, **121**, 8147-8153

*Ind. Eng. Chem. Res* (2.843)

Tamaghna Chakraborti and Jhumpa Adhikari, Phase Equilibria and Critical Point Predictions of Mixtures of Molecular Fluids Using Grand Canonical Transition Matrix Monte Carlo, Ind. Eng. Chem. Res., 2017, **56** (22), pp 6520-6534, DOI: 10.1021/acs.iecr.7b01114

*Condensed Matter* (2.649)

Dimple, Nityasagar Jena and Abir De Sarkar, Compressive strain induced enhancement in thermoelectric-power-factor in monolayer MoS2 nanosheet, Journal of Physics: Condensed Matter **29** (2017) 225501 (7pp)

Mit H. Naik, Manish Jain, Substrate screening effects on the quasiparticle band gap and defect charge transition levels in MoS2, Condensed Matter, Materials Science, arXiv:1710.09569

V. Ravi Chandra, Jyotisman Sahoo, The spin-1/2 Heisenberg antiferromagnet on the pyrochlore lattice: An exact diagonalisation study, Condensed Matter. arXiv:1710.11316

*J. Mat. Sci*(2.599)

V. Kumar and D. R. Roy, Structure, Bonding, Stability, Electronic, Thermodynamic Thermoelectric Properties of Six Different Phases of Indium Nitride, (Under Review) J. Mat. Sci. (Springer Link): JMSC-D-17-05053

*Materials Letters* (2.59)

Rajeev K and Dr. Radhakrishnan R, Electronic, Optical and Mechanical Properties of Lead-Free Halide Double Perovskites using First-Principles Density Functional Theory, Materials Letters

*Computers & Fluids* (2.313)

Rajesh Ranjan, S.M. Deshpande, Roddam Narsimha, New insights from high-resolution compressible DNS studies on an LPT blade boundary layer, Computer and fluids 153 (2017),49-60.

*J. Biomol. Struct. Dyn.* (2.300)

Shuaib, S.; Goyal, B. Scrutiny of the mechanism of small molecule inhibitor preventing conformational transition of amyloid42 monomer: insights from molecular dynamics simulations. J. Biomol. Struct. Dyn. 2017, DOI:10.1080/07391102.2017.1291363.

*J. Mol. Recognit.* (2.175)

Saini, R. K.; Shuaib, S.; Goyal, B. Molecular insights into A42 protofibril destabilization with a fluorinated compound D744: A molecular dynamics simulation study. J. Mol. Recognit.

2017, **30**, e2656.

*Materials Chemistry and Physics* (2.084)

K.C.Bhamu and K.R.Priolkar, Electronic and optical properties of AgAlO2: A first-principles study, Materials Chemistry and Physics, Volume 190, 1 April 2017, Pages 114-119

*Journal of Physics and Chemistry of Solids* (2.048)

Q.Mahmood, M.Hassan, S.H.A.Ahmad, K.C.Bhamu, Asif Mahmood, Shahid M.Ramay ,Study of electronic, magnetic and thermoelectric properties of AV2O4 (A = Zn, Cd, Hg) by using DFT approach, Journal of Physics and Chemistry of Solids (in press) https://doi.org/10.1016/j.jpcs.2017.08.007.

*EPL* (1.9)

Jalal Sarabadani, Bappa Ghosh, Srabanti Chaudhury and Tapio Ala-Nissila, Dynamics of end-pulled polymer translocation through a nanopore, EPL, **120**, 38004(2017)

*Molecular Physics* (1.837)

Siddheshwar Chopra and Felix Plasser, UV Absorption in metal decorated Boron nitride flakes: A theoretical analysis of excited states, Molecular Physics, **115**, 19, 2469-2477, (2017).

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*Journal of Molecular Graphics and Modeling* (1.754)

Manan Desai, Neeraj Gaur and Debjani Dasgupta, Effect of temperature of structural stability of FtsZ from E.coli and P.abyssi: A comparative study, Journal of Molecular Graphics and Modeling (Review)

*Int. J. Mass Spectromet* (1.702)

Y. Krishnan, P. Rajbangshi and M. Paranjothy, Theoretical Study of Perbenzoate Anion Decomposition Pathways in the Gas Phase, Int. J. Mass Spectromet. 2017 (In press).

*Journal of Modern Physics B* (1.669)

P. S. Thokal and Pradip B Shelke, MAGNETIC PROPERTIES OF PATTERNED THIN ISING FILMS, (submitted) Journal of Modern Physics B (world Scientific Publishers, Singapore)

*J. Chem. Sci.* (1.2998)

Y. Krishnan, A. Vincent and M. Paranjothy, Classical Dynamics Simulations of Interstellar Glycine Formation via CH2=NH + CO + H2O Reaction, J. Chem. Sci. 2017, **129**, 1571 1577.

*Nanoscience & Nanotechnology* (1.25)

Siddheshwar Chopra,Exciton Size and Natural Transition Orbital Investigation in Varied Graphene Forms: High Level Ab-intio Computations, doi:10.2174/2210681207666170407165919, Nanoscience & Nanotechnology-Asia, 7, 2017.

*Meteorology and Atmospheric Physics* (1.159)

Sumita Kedia, Ramesh K. Vellore, Sahidul Islam, and Akshara Kaginalkar, A study of Himalayan extreme rainfall events using WRF-Chem, Meteorology and Atmospheric Physics (submitted)

*Theoretical and Computational Fluid Dynamics* (1.097)

Yogesh Prasaad Madras Sethuraman, Johan Larsson, and Krishnendu Sinha, Thermodynamic Fluctuations in canonical shock-turbulence interaction, (under review) Theoretical and Computational Fluid Dynamics journal, submitted.

*Astronomische Nachrichten* (0.916)

Brandenburg A. and Chatterjee, P, Strong nonlocality variations in a spherical mean-field dynamo, 2018, to appear in Astron Nachr (eprint arXiv:1802.04231)

*Computers & Geosciences* (0.70)

Rastogi, R., Londhe, A., Srivastava, A., Sirasala, K., Khonde, K., 2017, 3D Kirchhoff depth migration algorithm: A new scalable approach for parallelization on multicore CPU based cluster, Computers & Geosciences (Elsevier), **100**, 67-75.(IF : 0.70)

*Sect. B Biol. Sci* (0.67)

Kumar, A., Kumar, S., Kumar, A and MNVP Gajula. Homology Modeling, Molecular Docking and Molecular Dynamics Based Functional Insights into Rice Urease Bound to Urea, Proc. Natl. Acad. Sci., India, Sect. B Biol. Sci. PP1-10, 2017.

*Pramana - Journal of Physics* (0.52)

Dimple, Nityasagar Jena, Shounak Dhananjay Behere and Abir De Sarkar, "The effects of different possible modes of uniaxial strain on the tunability of electronic and band structures in MoS2 monolayer nanosheet via first-principles density functional theory", Pramana - Journal of Physics - Springer, **89**(2017)1-7 (IF : 0.52)

Advances in Computation, Modeling and Control of Transitional and Turbulent Flows (book) Rajesh Ranjan, S.M.Deshpande and Roddam Narasimha, a High-Resolution Compressible DNS Study of Flow Past a Low-Pressure Gas Turbine Blade, 2016.

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# 8

# Visits

Total number of visitors during Mar. 20,2017 - Feb. 21,2018 : 2750

**Visits by dignitaries**

- Lieutenant General. Anil Kapoor , VSM, Director General of information System, Indian Army, India .
- Prof. E. Saibaba Reddy, Former Vice Chancellor, VSSUT, Burla ,Odisha.
- Mr. S. B. Mahajan , AO, ICISA, Noida, UP.
- Mr. S. M. Dongaswar, AAO, ICISA, Noida, UP.
- Mr. Dilip Kumar Naik, Sr.AO, , ICISA, Noida, UP
- Shri. Reji Nair , STQC, Triruvanthapuram.
- Shri. V. P. Sharma, former Director Technical Services, Cisco Systems, Bangalore and Mumbai.
- Ms. R. Uma, Dy. Director, P& T Audit Office, Mumbai.
- Dr. S. N. Bhaskar, Director ,NTRO ,Delhi.
- Shri. Aman Kumar, NTRO, Delhi.
- Prof. K. K. Shukla, IIT(BHU),Varanasi, UP.
- Mr. Ramiro Wahrhaftig, Brazil.
- Prof.Miguel Matrakas,Brazil.
- Mr.Luiz Felipe Kraemer Carbonell, Brazil.
- Mr. Daniel Ferreira,CTI, Brazil.
- Mr. Chandrakant Ambadas Dhakare , Police Head Quarter, Pune.
- Mr. Konstantin Chebostaev, International Relations Manager, "Health Modeling Technologies" Vice-President for International Affairs of the National Association of Medical Informatics (NAMI), Moscow, Russia.

- Prof. Mikhail Natenzon, Chairman of Board of National Telemedicine Agency, Moscow, Russia.
- Mr. E Van, Advisor Director General, Portal RAMN, Asia-Pacific region.moscow, Russia.
- Mr. Kungurtsev Sergey, Head of the international and Interregional link division of the Department for Municipal affairs, Okrug , Russia.
- Shri. Krishna Murthy, Prog. Director, YASHADA, Pune.
- Mr. Md. Kamruzzaman, Deputy Secretary, Information & Communication Technology Division. Ministry of posts, Telecommunication and IT, Bangladesh.
- Dr. B. K. Panigrahy ,Registrar, IIIT- Naya Raipur.
- Dr. Pradeep K. Sinha, Vice Chancellor & Director, IIIT- Naya Raipur.
- Vice Admiral SN Ghormade, AVSM,NM, Director General of Navel Operations.
- Prof. D. N. Reddy, Director, CR Rao AIMSCS, HCU, Hyderabad.
- Dr. Ajay .K. Nayak , Joint Secretary, Govt of Odisha, Bhubaneswar.
- Prof. R. K. Singh, Dean (Students Welfare), MNNIT, Allahabad.
- Shri. M. Krishna, Assistant Director (DOC),Central Forensic Science Laboratory (CFSL ),Hyderabad.
- Wg Cdr A. Ahluwalia, Indian Air Force.
- Dr. Bahgat Sammakia, Interim President , SUNY Polytechnic Institute, New York.
- Shri. Jual Oram, Honble Minister of tribal affairs, Govt of India.
- Wg Cdr M.M. Ingale, Indian Air Force.

Table 8.1: Summary of Industrial Visits

| Institution | No. of visitors | Visit Date |
|---|---|---|
| **2017** | | |
| Govt. Poly Malvan | 40 | Mar. 20 |
| Universal college | 70 | Mar. 23 |
| Chhotubhai Gopalbhai Patel Institute of Technology | 50 | Mar. 30 |
| ITMUR-School of Engineering & Research, Raipur | 34 | Apr. 03 |
| Pimpri Chinchwad College of Engineering | 15 | Apr. 07 |
| Neotech technical campus, Vadodara | 86 | Apr. 10 |
| National College | 45 | Apr. 20 |
| SPPU | 25 | May 19 |
| JSPM Polytechnic | 150 | Jul. 4,5,6 |
| Trinity College | 50 | Jul. 13 |
| Govt.Poly.Pune | 60 | Jul. 14 |

*Continued on next page*

Table 8.1 – *Continued from previous page*

| Institution | No. of visitors | Visit Date |
|---|---|---|
| MGM Polytechnic Aurangabad | 64 | Jul. 14 |
| VPM's Polytechnic, Thane | 69 | Jul. 20 |
| VPM's Polytechnic, Thane | 80 | Jul. 20 |
| JSPM's JSCOE | 50 | Jul. 21 |
| Marathawada Mitra Mandals, polytechnic, pune | 50 | Jul. 28 |
| Regal College of Technology & Management, Kalyan | 50 | Aug. 10 |
| TMESICS, Mandvi | 70 | Aug. 11 |
| Nes Ratnam College, Mumbai | 50 | Aug. 17 |
| Jaywantrao Sawant Polytechnc, Hadapsar | 60 | Aug. 18 |
| NVPAS Vallabh vidyanagar, Gujrat | 60 | Aug. 22 |
| Smt. Geeta D. Tatkare Polytechnic, Gove-Kolad | 40 | Aug. 23 |
| Sinhgad Technical Education Society,RMDSSOE | 100 | Aug. 30-31 |
| CME Pune | 21 | Sep.6 |
| Amrutvahini College of Engineering, Sangamner | 56 | Sep. 07 |
| Pimpri Chinchwad Polytechnic, NIGDI | 120 | Sep. 13-14 |
| G V Acharya Polytechnic, Shelu-Karjat | 45 | Sep. 22 |
| Govt. Polytechnic Pune | 65 | Sep. 28 |
| AIT Pune | 20 | Oct. 4 |
| Government Polytechnic Pune | 134 | Oct. 5-6 |
| Pillai Arts Commerce and Science College | 176 | Oct. 10,12,17 |
| Pimpri Chinchwad College of Engineering | 20 | Oct. 30 |
| **2018** | | |
| St Francis College for Women, Begumpet | 50 | Jan. 9 |
| G. R. Patil College, Mumbai | 50 | Jan. 12 |
| Sarvajanik College of Engineering and Technology (SCET) | 100 | Jan.18-19 |
| Zeal Education Society Narhe, Pune | 120 | Jan. 23-24 |
| Sandip University, Nashik | 21 | Jan. 25 |
| MIT-WPU kothrud,Pune | 120 | Jan. 30-31 |
| Shree. Vatvriksha Swami Maharaj,Sholapur | 40 | Feb. 2 |
| D.Y. Patil College of Engineering & Technology, Kolhapur | 38 | Feb. 7 |
| Latthe Edn Soc, Sangli | 41 | Feb. 14 |
| Royal College of Science, Mira Road | 50 | Feb. 15 |
| SAL College of Eng and Tech Inst, Ahmedabad | 40 | Feb. 16 |
| G H Raisoni College of Engg | 30 | Feb. 16 |
| Dr Manoj Shette College of engineering Kasara | 25 | Feb. 21 |

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# Appendices

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# Appendix A

# Users across Institutions

**Below is the list of NPSF users across Institutions**

Table A.1: Users across Academic Institutions

| Academic Institutions | No. of Users |
|---|---|
| Ahmednagar College | 1 |
| Amity University | 2 |
| Aligarh Muslim University | 5 |
| Anna University | 2 |
| Army Institute of Technology, Pune | 5 |
| Bhusawal Arts, Sci. & PO Nahata Commerce College | 1 |
| BITS Pilani, Hyderabad Campus | 2 |
| CMR College of Engg. & Tech. | 2 |
| Carnegie Mellon University | 1 |
| College of Engineering, Pune | 6 |
| Central Univ. of Bihar | 1 |
| Central Univ. of Gujarat | 3 |
| Central University of Haryana | 3 |
| Central University of Rajasthan | 1 |
| Delhi University | 2 |
| Dibrugarh University | 3 |
| D. Y. Patil University,Navi Mumbai | 3 |
| Gandhi Institute of Tech. and Mgmt., Hyderabad | 1 |
| GLA University, Mathura | 1 |
| Goa University, Goa | 2 |
| Govt. College, Tonk | 1 |
| Guru Nanak Dev University | 1 |
| Gujarat Technological University | 1 |
| HPT Arts & RYK Science College | 1 |
| Himachal Pradesh University | 5 |
| IIA, Bangalore | 12 |

*Continued on next page*

Table A.1 – *Continued from previous page*

| Academic Institutions | No. of Users |
|---|---|
| IIIT, Hyderabad | 4 |
| IIIT, Delhi | 4 |
| IIIT, Madhya Pradesh | 4 |
| IISc, Bangalore | 7 |
| IISER, Pune | 59 |
| IISER, Mohali | 1 |
| IISER, Thiruvananthapuram | 3 |
| IIT Bombay | 226 |
| IIT Bhubaneswar | 2 |
| IIT Delhi | 8 |
| IIT(ISM) Dhanbad | 2 |
| IIT Guwahati | 24 |
| IIT Gandhinagar | 10 |
| IIT Hyderabad | 30 |
| IIT Jodhpur | 12 |
| IIT Kanpur | 23 |
| IIT Kharagpur | 12 |
| IIT Patna | 8 |
| IIT Roorkee | 5 |
| IIT Ropar | 8 |
| INST, Mohali | 22 |
| JMI University | 3 |
| Jiwaji University | 3 |
| JSPM-TSSM Space Research Programme | 1 |
| JNU | 2 |
| Kurukshetra University | 3 |
| Manipal University | 2 |
| MIT Pune | 1 |
| NIT Calicut | 1 |
| NIT Rourkela | 1 |
| NIT Silchar | 1 |
| Panjab University | 2 |
| PJTSAU, Hyderabad | 1 |
| PDU Shekhawati Univ., Sikar | 1 |
| PU College, Mizoram | 1 |
| PVPIT Pune | 3 |
| RTM Nagpur University | 2 |
| SASTRA University, Thanjavur | 3 |
| Shekhawat University | 1 |
| SRM University | 3 |

*Continued on next page*

Table A.1 – *Continued from previous page*

| Academic Institutions | No. of Users |
|---|---|
| SRTM University | 2 |
| St. Xavier's College, Ahmedabad | 1 |
| S P Pune University | 36 |
| Sri Guru Granth Sahib World University | 9 |
| SVNIT Surat | 4 |
| Symbiosis Institute of Technology, Pune | 1 |
| Tetrahydrix Engg. Pvt. Ltd. | 1 |
| University of Hyderabad | 1 |
| University of Madras | 1 |
| University of Rajasthan | 1 |
| VNIT Nagpur | 10 |
| Whistling Woods International Institute | 2 |
| **Total** | **646** |

Table A.2: Users across research institutions

| Research Institutions | No. of Users |
|---|---|
| BARC, Mumbai | 1 |
| CBS, Mumbai | 2 |
| CIFRI, Kolkata | 2 |
| C-DAC | 137 |
| CSIR, Delhi | 4 |
| CSIR, Indore | 1 |
| DRDO-BU Centre for Life Sciences, Coimbatore | 4 |
| E-teacher | 2 |
| GARUDA | 165 |
| HRI, Allahabad | 2 |
| IACS Kolkata | 1 |
| IASST, Guwahati | 4 |
| INDO KOREA Science and Technology Center | 1 |
| Indian Air Force, Banglore | 1 |
| ISRO | 5 |
| ISc Mumbai | 2 |
| IUCAA, Pune | 7 |
| JNCASR, Bangalore | 11 |
| NABI, Mohali | 1 |

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Table A.2 – *Continued from previous pae*

| Research Institutions | No. of Users |
|---|---|
| NCL, Pune | 8 |
| NCRA, Pune | 6 |
| NIC | 2 |
| NISER | 2 |
| PRL, Ahmedabad | 3 |
| RRI, Bangalore | 3 |
| SINP, Kolkata | 2 |
| THSTI | 4 |
| Vijay Kumar Foundation, Gurgaon | 7 |
| **Total** | **390** |

# Appendix B

# Projects Enrolled during Year 2017-18

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 B.1: Projects using NPSF Yuva II compute time

| Institution | Project | Chief Investigator | No. of users |
|---|---|---|---|
| Ahmednagar college, Ahmednagar | To study the propertiees of layered structures and effects of doping there in using density functional theory | Dr. Pradip B. Shelke | 1 |
| Amity University,Noida | DFT based chemical, structural, optical and magnetic study of functionalized Graphene nanoribbons | Dr. Siddheshwar Chopra | 1 |
| Bhusawal Arts, Science And P. O. Nahata Commerce College | Quantam Chemical Investigations on Phenyl-Acetylene Clusters | Dr. Sachin D. Yeole | 1 |
| CDAC Banglore | SuMegha is a scientific cloud which can provision on-demand access to shared pool of virtual HPC resources easily as and when needed by the HPC applications | Dr. B Arunachalam | 1 |
| CDAC Pune | IoE Test-bed as Smart City Solutions for Disaster Management and Video Surveillance | Dr. Sanjay Kadam | 1 |
| Central University of Haryana | Ab initio Molecular Dynamics simulation of Ionic Liquid doped Polymer Electrolyte Membranes and Platinum Electrode Interface | Dr. Anurag Prakash Sunda | 3 |
| Central University of Rajsthan | Tailoring the electronic properties of surface/interface of semiconductor oxides | Dr. Divya Srivastava | 1 |
| College of Engineering Pune | Blockchain Scaling and Measuring the Variation in Latency as the Network Scalability Changes | Prof. Jimi Abraham | 4 |
| Consortium for Scientific Research, Indore | First Principles Modeling of Dzyaloshinskii-Moriya Interactions in Magnetic Multilayers | Dr. Rajamani Raghunathan | 1 |
| Dibrugadh University | Aerosol Radiative forcing over India(ARFI) and Atmospheric Trace gases, Chemistry, Transport and Modeling(AT-CTM) | Dr. Binita Pathak | 3 |
| Harish-Chandra Research Institute, Jhunsi | Magnetic switching using 3d-organometallic molecule | Prof. Prasenjit Sen | 2 |

*Continued on next page*

Table B.1 – *Continued from previous page*

| Institution | Project | Chief Investigator | No. of Users |
|---|---|---|---|
| Himachal Pradesh University | In-plane heterostructure of Transition metal dichalcogenides | Dr. Raman Sharma | 2 |
| H.P.T Arts and R.Y.K. Science College, Nasik | Theoretical investigation of structural, electronic, magnetic and optical properties of undoped and doped iron oxide nanostructures. | Dr. Dattatraya Laxman Lalsare | 1 |
| Indian Association for the Cultivation of Science, Kolkata | Computational Investigations for the Linear and Nonlinear Optical Properties of Metal and Covalent Organic Frameworks: Applications for Detection of Molecules | Dr. Ayan Datta | 1 |
| Indian Institute of Information Technology and Management, Gwalior, MP | High energy density Supercapacitors and Effective Gas/Chemical/Bio-Sensors using 2D/1D Materials | Dr. Anurag Srivastava | 4 |
| International Institute of Information Technology, Hyderabad | Simulation of Fault Motion Analysis, Simulation of Collapse behavior of buildings subjected to Earthquakes | Dr. Ramancharala Pradeep Kumar | 4 |
| IISER Pune | Unconventional phase transitions in classical cubic dimer model Emergent SO(5) symmetries | Dr. Sreejith Ganesh Jaya | 1 |
| | Point-Defects in Two-Dimensional Materials | Dr. Mukul Kabir | 3 |
| | Role of Magnetism in Mn-Rich Steels | Dr. Mukul Kabir | 2 |
| | Catalyst design for molecular-H splitting | Dr. Mukul Kabir | 2 |
| | Vacancy diffusion in graphene | Dr. Mukul Kabir | 1 |
| | Microscopic mechanism for methane hydrate formation | Dr. Mukul Kabir | 2 |
| | O2 molecule splitting and diffusion on LaMnO3 surface | Dr. Mukul Kabir | 2 |
| | Study of CdS and CdTeS quantum dots decorated on TiO2 nanowires | Dr. Prasenjit Ghosh | 7 |

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Table B.1 – *Continued from previous page*

| Institution | Project | Chief Investigator | No. of Users |
|---|---|---|---|
| | Selective hydrogenation of acetylene to ethylene on PdGa surfaces and clusters supported on MgO | Dr. Prasenjit Ghosh | 7 |
| | Molecular Modelling and Dynamics of Polymers, Gas hydrates and ionic liquids: An alternative energy initiative | Dr. Arun Venkatnathan | 5 |
| IIT Guwahati | Atomistic Simulation of Fast Ion Transport in Solids | Dr. Padma Kumar Padmanabhan | 5 |
| | Molecular Dynamics Study of Allosteric Modulation and Regulation of the HIV-1 restriction factor, SAMHD1 | Dr. Swati Bhattacharya | 2 |
| IIT Hyderabad | Investigating seismic source physics inclusion into Engineering analysis of Built-Environment | Dr. Surendra Nadh Somala | 6 |
| | Calorimetric detection of UCHLI | Dr. Anindya Roy | 3 |
| | Structure and dynamics of RMA duplexes comprising trinucleotide repeat expansion | Dr. Thenmalarchelvi Rathinavelan | 5 |
| IIT ISM | Three Dimensional modelling of Magnetotelluric Data over Dalma and Dhanjori Volcanics | Prof. Shalivahan | 2 |
| IIT Jodhpur | Direct Numerical Simulation of partially premixed Tabular Flames | Dr. Sudipto Mukhopadhyay | 1 |
| | Computational investigation of the nature of active sites of Ni/CeO2 catalyses | Dr. Sriram Goverapet Srinivasan | 1 |
| | Chemical Dynamics Simulations of Complex Organic Reactions: Mechanistic Insights and Microsolvation Effects | Dr. Manikandan Paranjothy | 2 |
| IIT Patna | Development of Smart Materials using Molecular Dynamics Simulation | Dr. Sandip Khan | 3 |
| IIT Roorkee | Impact of LULC and climate change in a Himalayan basin | Dr. C. S. P. Ojha | 2 |

*Continued on next page*

Table B.1 – *Continued from previous page*

| Institution | Project | Chief Investigator | No. of Users |
|---|---|---|---|
| | A molecular dynamics based atomistic simulation to study the effect of nanofillers in the mechanical and thermal properties of polymer based nanocomposites | Prof. Avinash Parashar | 2 |
| | Large-Scale Atomistic Molecular Dynamics study of drug release from stimuli-responsive polymeric carriers | Dr. Prateek Kumar Jha | 1 |
| INST, Mohali | Electronic and magnetic properties of oxide interface and super latices | Dr. Chandan Bera | 3 |
| | Quantum capacitance calculation of carbonaceous materials | Dr.Ramendra Sundar Dey | 2 |
| | Atomic scale design of novel nanomaterials for clean energy and devices | Dr. Abir De Sarkar | 6 |
| | Ab initio molecular dynamics (AIMD) Simulations | Dr. Md. Ehesan Ali | 1 |
| | (Institute of Nano Science and Technology) Electronics and Thermal Properties of chalcogenide | Dr. Chandan Bera | 2 |
| Jamia Millia Islamia University, New Delhi | First Principle study of the electronic structures of heterostructure devices and their related applications | Dr. Anver Aziz | 2 |
| Jawaharlal Nehru Centre for Advanced Scientific Research, Banglore | Modelling of supermolecular polymers | Prof. Balasubramanian Sundaram | 1 |
| JSPM-TSSM Space Research Programme | Space Research Programme | Prof. Dr. Srinivas Narasimha Kini | 1 |
| Kurukshetra University, Haryana | Simulations of rare earth free magnetic inorganic halide perovskites for photovoltaic applications | Dr. Manish Kumar Kashyap | 3 |
| National Institute of Science Education and Research, Odisha | Numerical Studies of correlated phases and transitions in frustrated magnets | Mr. V. Ravi Chandra | 1 |

*Continued on next page*

Table B.1 – *Continued from previous page*

| Institution | Project | Chief Investigator | No. of Users |
|---|---|---|---|
| | Biomolecular simulation: Molecular mechanism of signal transduction, protein-protein interaction and allosteric regulation | Dr. Suman Chakrabarty | 1 |
| NIT Silchur | Spectral element methods for elliptic and parabolic interface problems | Dr. Pankaj Biswas | 1 |
| Padmabhooshan Vasantdada Patil Institute of Technology, Pune | Direct numerical simulation of SDBD plasma actuation on flow separation for a circular cylinder | Dr. Pramodkumar Bagade | 3 |
| SASTRA University | Hydrogen Storage on Alkali Metal Functionalized Porous Descrete Organic | Dr. Venkataramanan N S | 2 |
| SP Pune University | Effect of substitutional doping on electronic structure of II-VI semiconductor quantum dots | Prof. Anjali Kshirsagar | 2 |
| | Computational Study on Graphene based NanoSheets for sensor applications | Dr Mrinalini Deshpande | 2 |
| | Electronic Properties of TM doped ZnO Sheet: Density Functional Study | Dr Mrinalini Deshpande | 4 |
| | Probing noncovalent interactions in Ionic Liquids using density functional theory | Prof. Shridhar P Gejji | 5 |
| Sri Guru Granth Sahib World University, | Design, Synthesis and Evaluation of Modified Short Peptides as Inhibitors of Amyloid-B (AB) Peptide Aggregation | Dr. Deepti Goyal | 5 |
| SVNIT, Surat | Development of Novel Cluster Assembled Materials from Potential Cluster Motifs: A New Insight under Density Functional Investigation | Dr. Debesh R. Roy | 4 |
| Symbiosis Institute of Technology, Pune | Water Quality Modeling of Lakes using Integrated Satellite Data Fusion | Mr. Rushikesh Kulkarni | 1 |

*Continued on next page*

Table B.1 – *Continued from previous page*

| Institution | Project | Chief Investigator | No. of Users |
|---|---|---|---|
| University of Madras | Studies on hybrid organicinorganic Halide Perovskite using first-principles density functional theory | Dr. R. Radhakrishnan | 1 |
| Vijay Kumar Foundation | Research work on nano-materials | Dr. Vijay Kumar | 7 |
| Visvesvaraya National Institute of Technology, Nagpur | First priniciple study of some topological materials | Dr. Poorva Singh | 2 |
| Whistling Woods International Institute | Rendering some of the shots for 15 Minute Short Film on PARAMYuva-II GPUs | Ms. Anuradha Bhatia | 2 |

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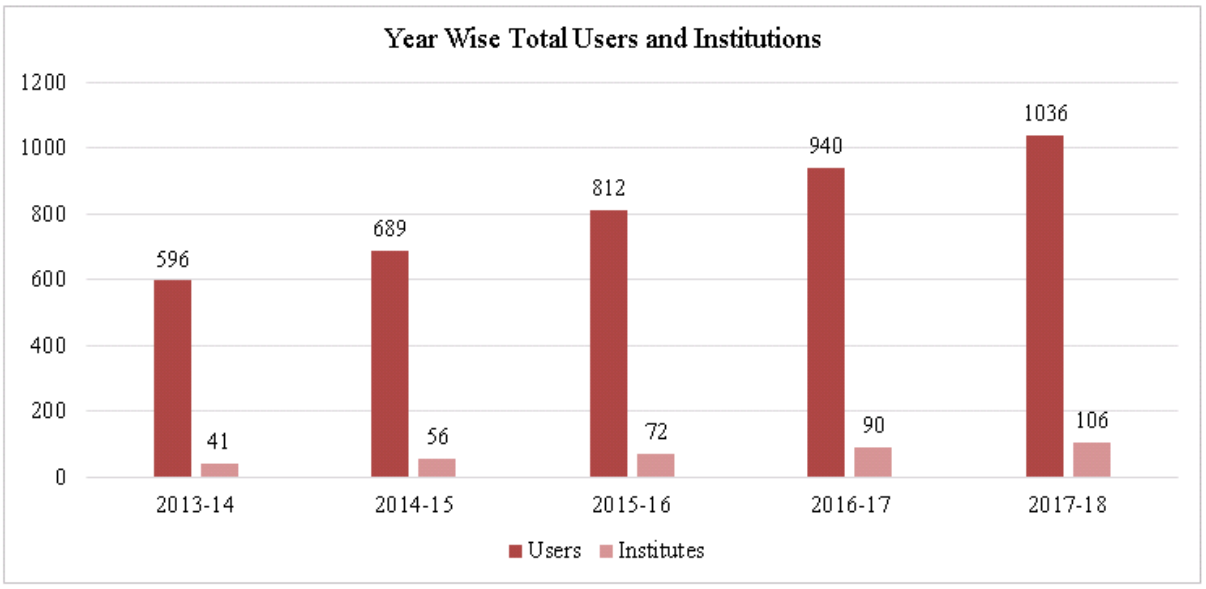
# Appendix C

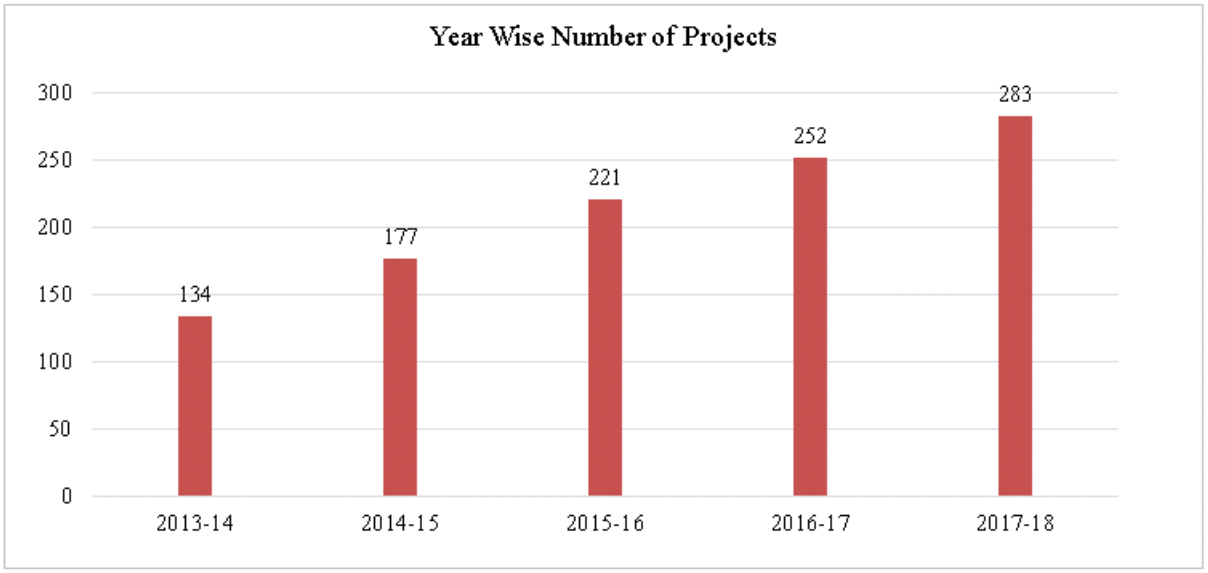
# Last Five Years at Glance

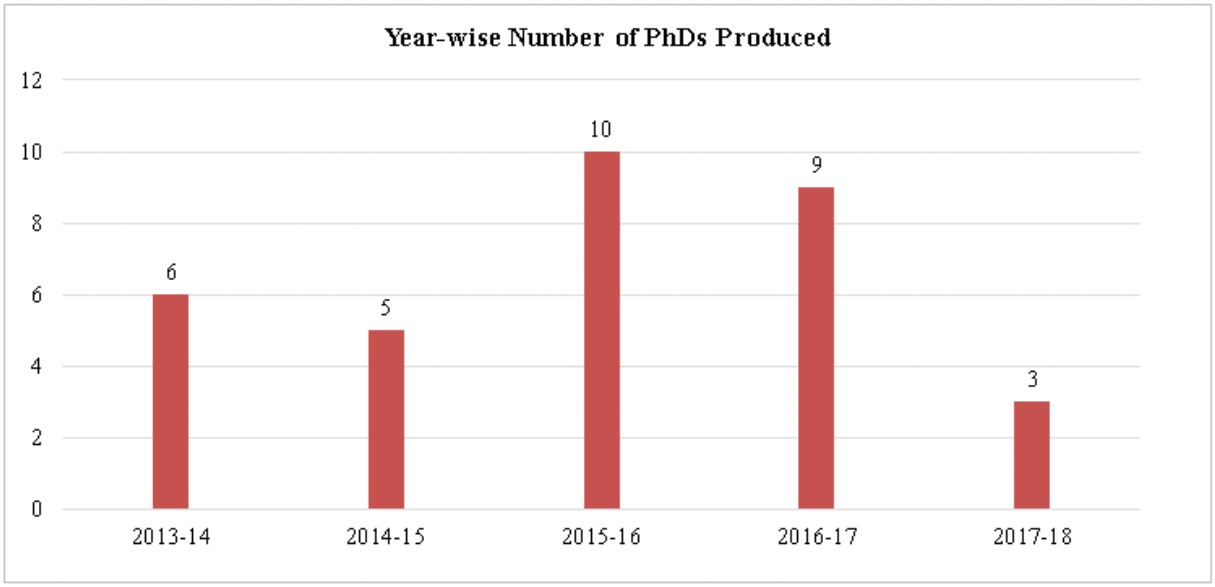
Below are some of the NPSF statistics of last five years i.e Year 2013-18.

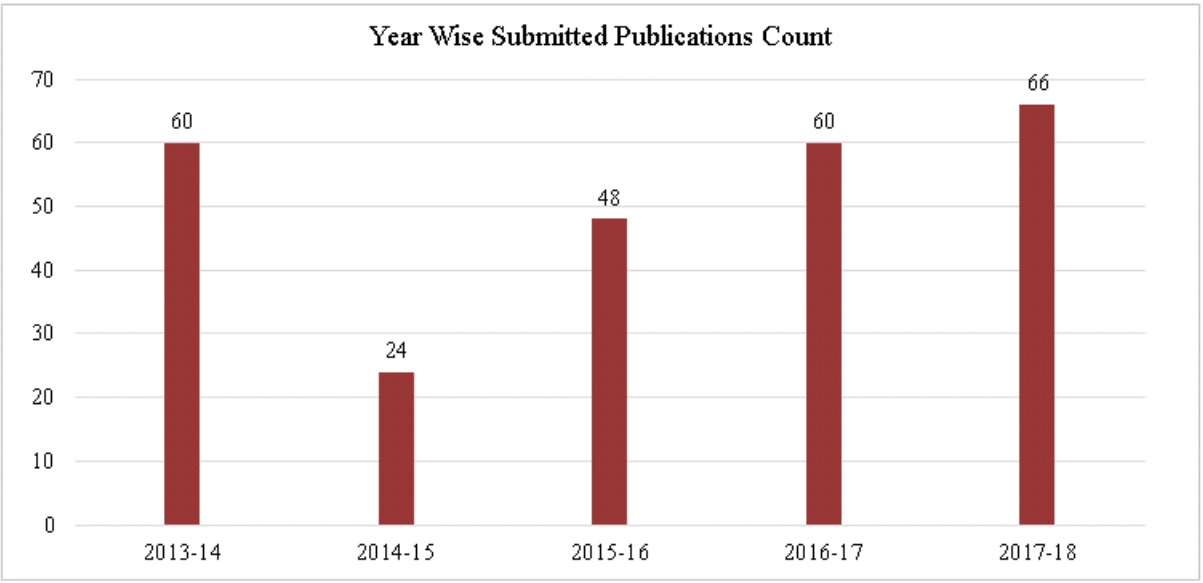
The statistics includes variation in cluster utilization, year-wise total number of projects, number of Ph.Ds & publications produced using NPSF.

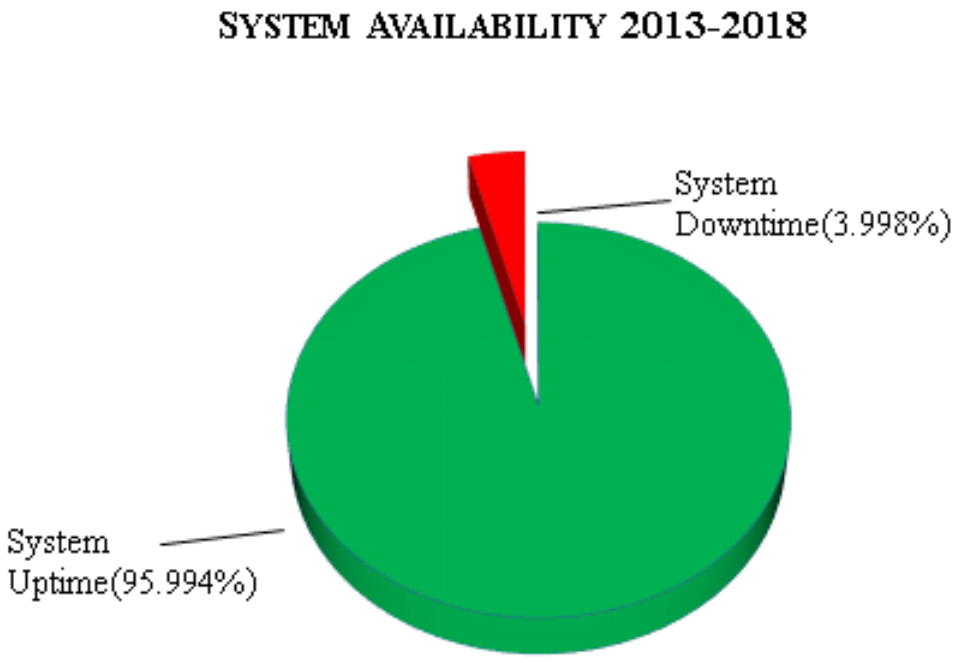
1. **2,67,617** Jobs completed processing.
2. **1036** Users.
3. **106** Institutions.
4. **283** Projects.
5. **33** Completed Ph.Ds.
6. **245** Publications.
7. **225** Total Ph.D. Students.

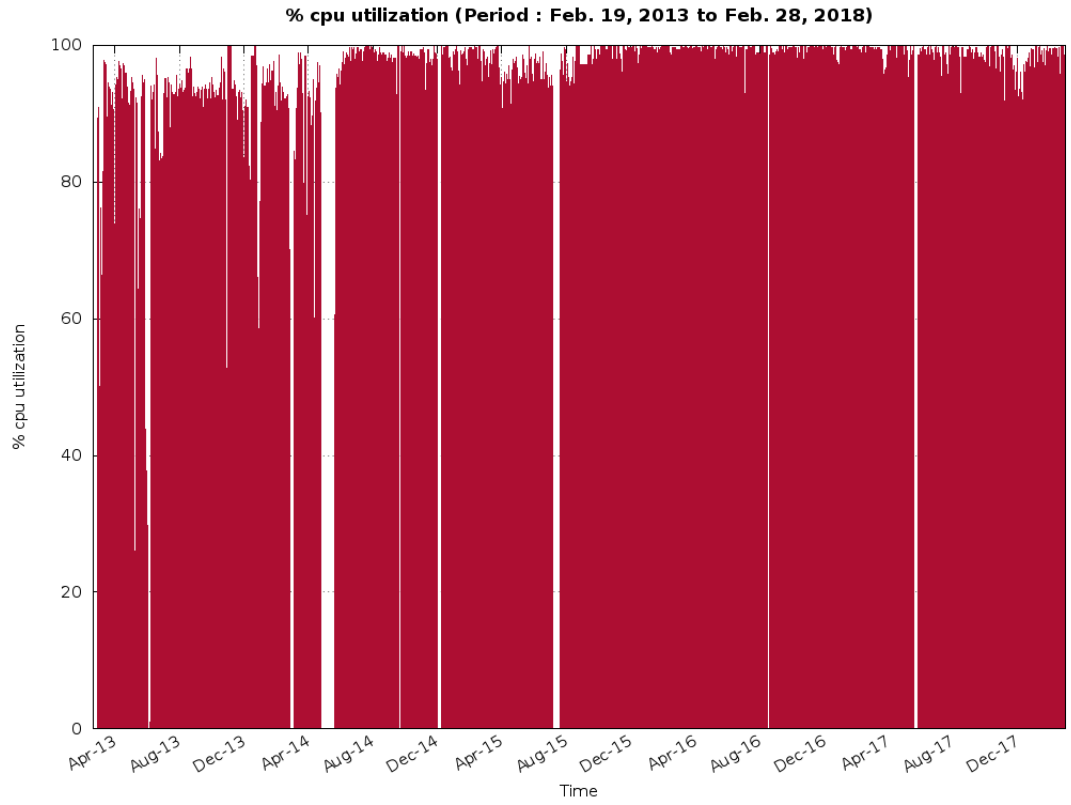

Year Wise Total Users and Institutions
1200
1000
800
600
400
200
0
596
41
689
56
812
72
940
90
1036
106
2013-14
2014-15
2015-16
2016-17
2017-18
Users
Institutes

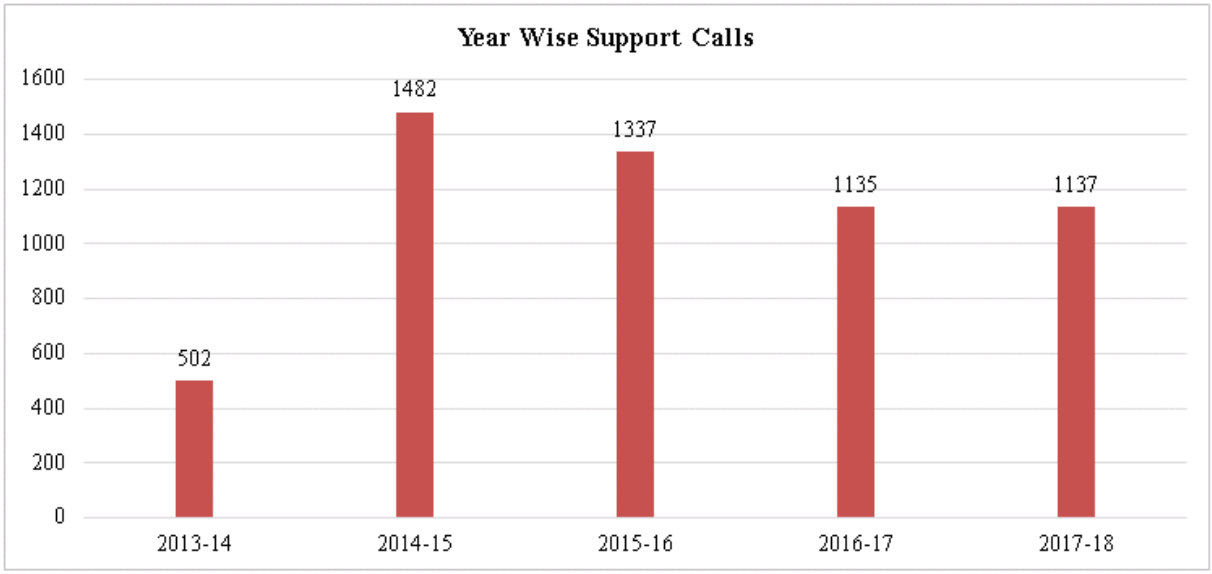

Year Wise Number of Projects
300
250
200
150
100
50
0
134
177
221
252
283
2013-14
2014-15
2015-16
2016-17
2017-18


Year-wise Number of PhDs Produced
12
10
8
6
4
2
0
6
5
10
9
3
2013-14
2014-15
2015-16
2016-17
2017-18


Year Wise Submitted Publications Count
70
60
50
40
30
20
10
0
60
24
48
60
66
2013-14
2014-15
2015-16
2016-17
2017-18


SYSTEM AVAILABILITY 2013-2018
System Downtime(3.998%)
System Uptime(95.994%)

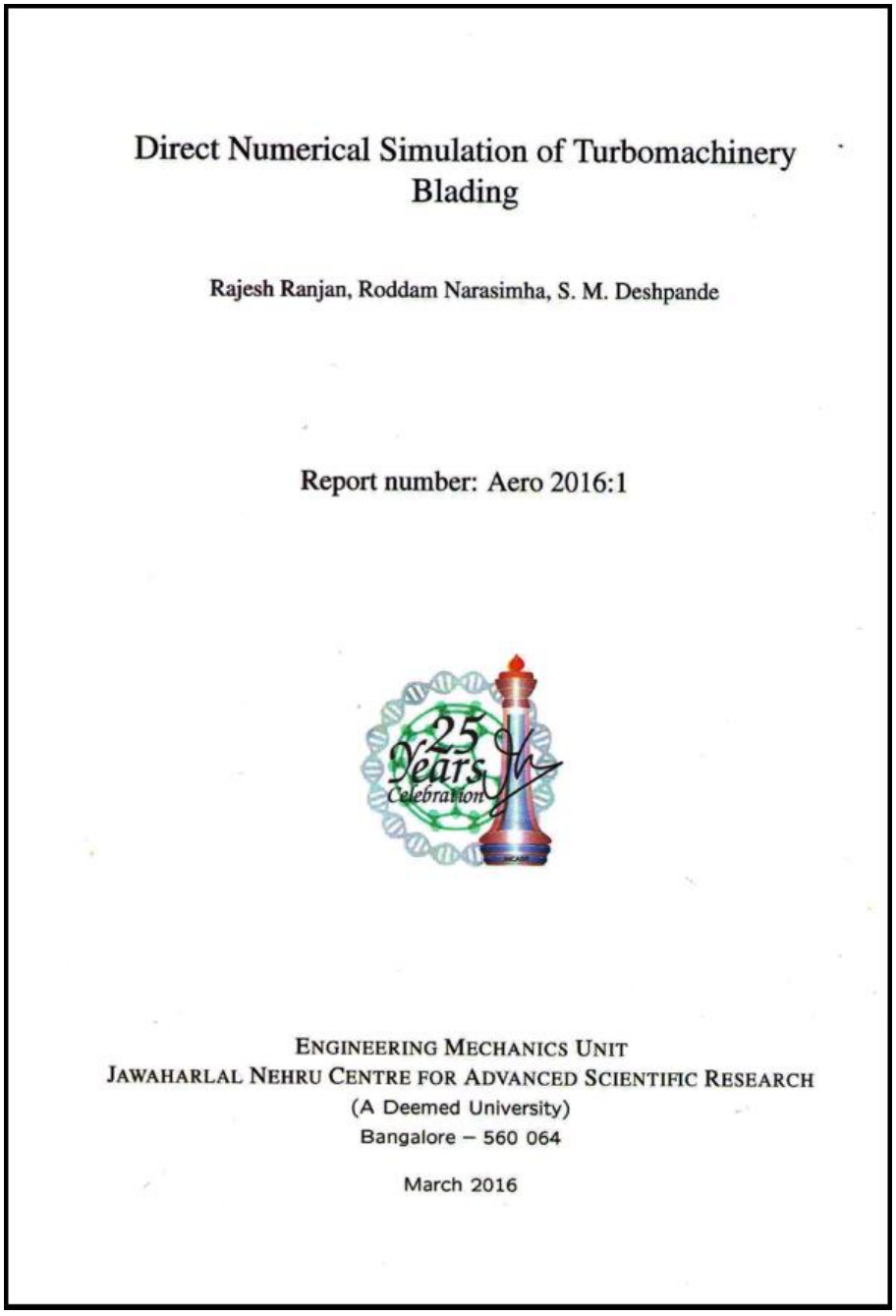

% cpu utilization (Period : Feb. 19, 2013 to Feb. 28, 2018)
% cpu utilization
100
80
60
40
20
0
Apr-13
Aug-13
Dec-13
Apr-14
Aug-14
Dec-14
Apr-15
Aug-15
Dec-15
Apr-16
Aug-16
Dec-16
Apr-17
Aug-17
Dec-17
Time


Year Wise Support Calls
1600
1400
1200
1000
800
600
400
200
0
502
1482
1337
1135
1137
2013-14
2014-15
2015-16
2016-17
2017-18

# Appendix D

# Users Appreciations

**Below are few of the user's appreciation quotes**



Direct Numerical Simulation of Turbomachinery Blading

Rajesh Ranjan, Roddam Narasimha, S. M. Deshpande

Report number: Aero 2016:1

ENGINEERING MECHANICS UNIT
JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
(A Deemed University)
Bangalore – 560 064

March 2016

## Acknowledgements

The work described in this report has been carried out as part of a project on *Direct Numerical Simulation of Turbo-Machinery blading*, sponsored through a grant from the GATET at Gas Turbine Research Establishment (GTRE) under the project "GTRE/GATET/CS15/1214/58" (JNCASR Project No. "RN/GTRE/4310"). The Principal Investigator Prof. Roddam Narasimha, and the Co-Principal Investigator Prof. S. M. Deshpande, are grateful for this support. The authors thank **Dr. C P Ramanarayanan**, Director, GTRE and **Dr. S. Kishore Kumar**, Associate Director, GTRE at the time of the award of this project. The authors would also like to express their gratitude to **Dr. M.Z. Siddique**, Present Director, GTRE for his continued support, and **Dr. K. V. L. Rao**, Technical Advisor, GTRE for his guidance throughout the project. The authors thank **Dr. Sivaramakrishna G.**, Programme Director, GATET, GTRE for his keen interest in the progress of the project, and his colleagues at GTRE for their support.

The authors would like to thank **Prof. Wolfgang Rodi, Dr. Jan Wissink, and Mr. Stephan Stotz** for providing important data on the blade and wake, and **Prof. O. N. Ramesh** for data pertaining to the simulation of free-stream turbulence. The authors sincerely acknowledge **Dr. Sukumar Chakravarthy** and his team at Metacomp Technologies, USA for providing the CFD++® license for scientific study.

This work would not have been possible without the generous co-operation and support received from C-DAC, Pune and CSIR-4PI, Bangalore. At C-DAC, the authors are grateful to **Dr. Rajat Moona**, Director General C-DAC and **Mr. Sanjay Wandhekar**, Associate Director and HoD, National PARAM Supercomputing Facility (NPSF) for their enthusiastic support. The authors thank the C-DAC support team specially Mr. Pankaj, Ms. Nisha, Mr. Gaurav, and Ms. Chaitali. At CSIR-4PI, the authors thank **Mr. Shyam Chetty**, Director NAL & Head CSIR-4PI for making their facilities available, and **Mr. R P Thangavelu**, in-charge of the supercomputing facility at CSIR-4PI for help regarding operational questions at the centre.

*"The reason we were not using CDAC account is because I recently moved out of JNCASR, and also because we shifted to doing simulations using GPUs. However, Param YUVA II was extremely useful initially in getting some important data for our research. I am sure for the CPU codes, it is one of the fastest supercomputer available in the country, and our colleague shall be using these accounts for cloud simulations."*

**Mr. Rajesh Ranjan,**
**Prof. Roddam Narasimha (Chief Investigator)**
**JNCASR, Banglore**

*"We have completed all the testing and designed simulations using the HPC facility ParamYuva-II. The facilities and whole hearted support rendered by NPSF has indeed played a significant role in completion of job. We sincerely wish to appreciate and grateful for the efforts put-in by the entire admin and help team. "*

**Mr. Ram Singh,**
**Dr. Krishna AchutaRao (Chief Investigator)**
**IIT Delhi, New Delhi**

*" I would like to convey my deep appreciation for your continuous support and assures you that your support has gone well in making some good scientific contributions and training of some people. We aspire to continue this journey and look forward to your continuous support."*

**Dr. Vijay Kumar (Chief Investigator)**
**Founder President,**
**Dr. Vijay Kumar Foundation, Gurgaon**

*"We are grateful for the assistance offered by C-DAC towards the project "CFD Analysis of 120 mm. FSAPDS Tank Ammunition" carried out by Centre for Modeling and Simulation, SPPU with DRDO. This project was successfully completed in 2016. The results have been reported to DRDO but cannot be shared in any academic journal. This note can serve as an acknowledgement of the computing support provided by C-DAC to test supersonic compressible flow simulations. "*

**Mr. Sukratu Barve,**
**Dr. Anjali kshirsagar (Chief Investigator)**
**S P Pune University, Pune**

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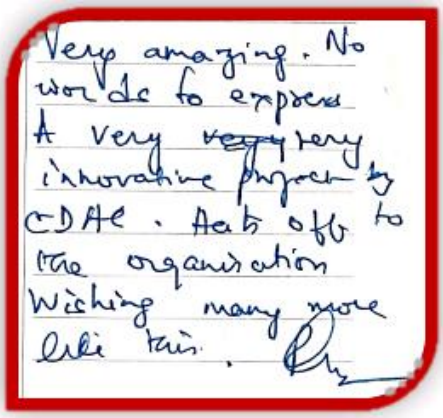
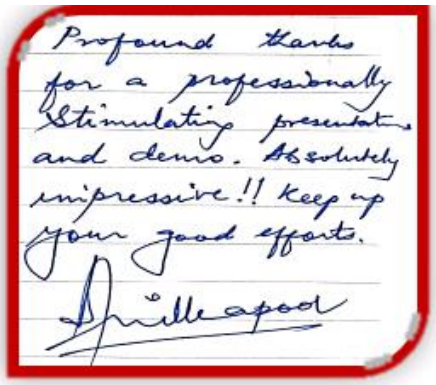
# Appendix E

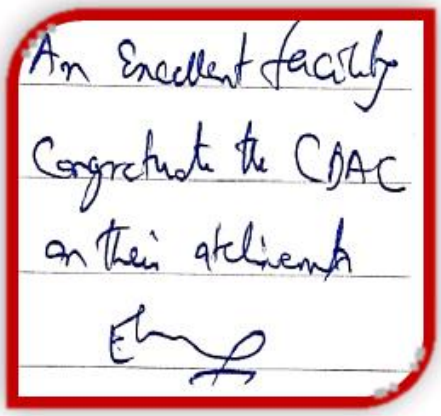
# Visitors Quotes



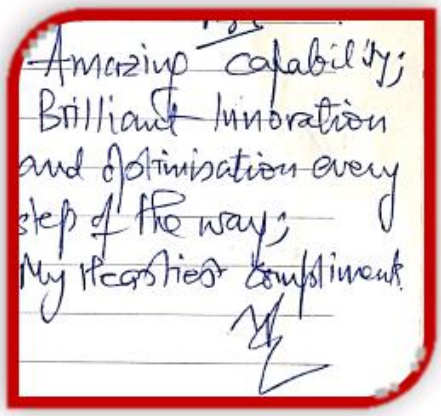

Ms. R. Uma, Dy. Director P&T Auditor, Mumbai



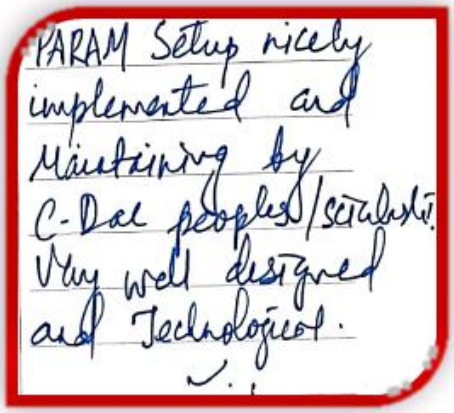

Lt. Gen Anil Kapoor, VSM, Director General, Information System, Indian Army, India.




Prof. E. Saibaba Reddy, Former VC, VSSUT, Barla, Odisha.

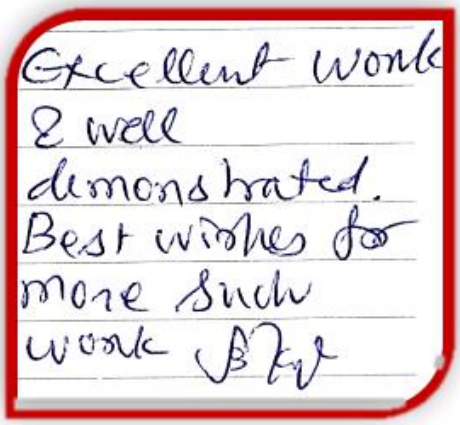



Shri. V. P. Sharma, Former Director (Technical Services), Cisco Systems, Mumbai.



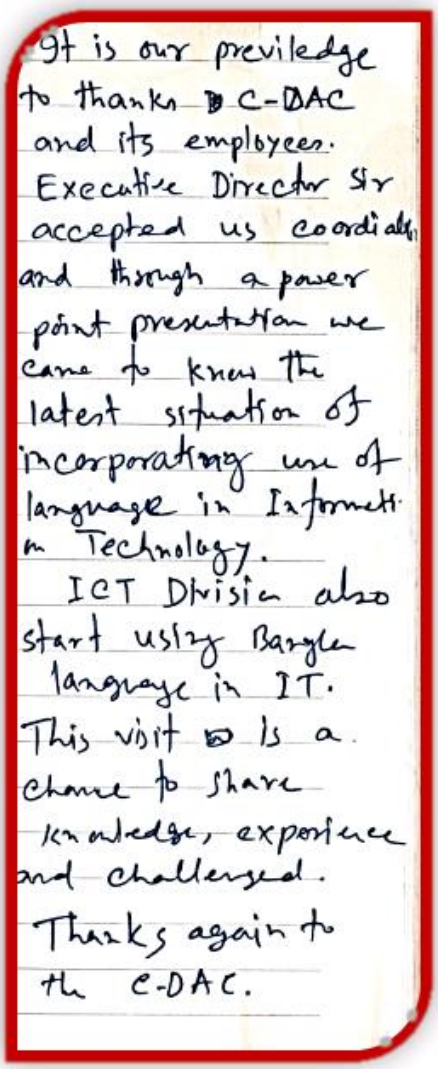

Shri. Chandrakant Ambadas Dhakare,
Police Head Quarter, Pashan Road, Pune


Prof. Mikhail Natenzon, Chairman, National
Telemedicine Agency, Moscow, Russia.

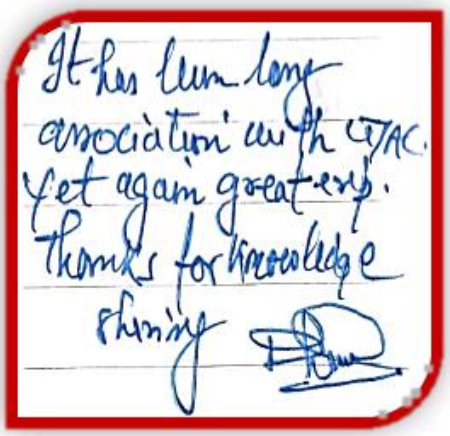



Shri. B. Krishna Murthy, Program Director,
Yashada, Pune


Wg Cdr M.M. Ingale, Indian Air Force.

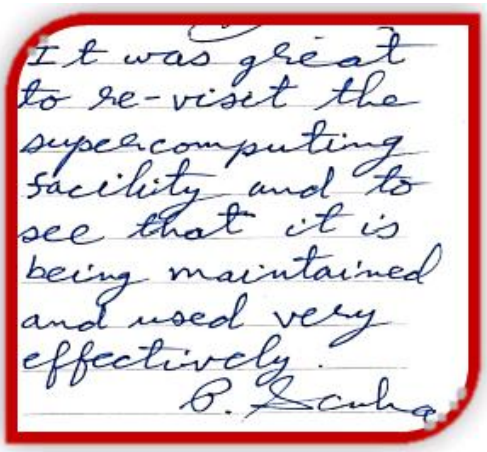



Md. Kamruzzaman ,Deputy Secretary,
Information & Communication Technology Division.
Ministry of Post & Telecom and IT,
Bangladesh.

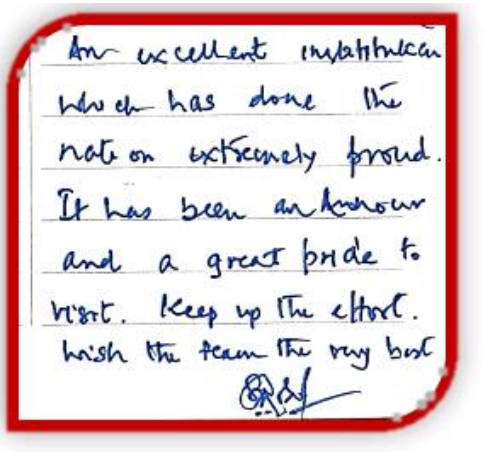



Dr. Dhananjay Srivastava, NTRO, Delhi.

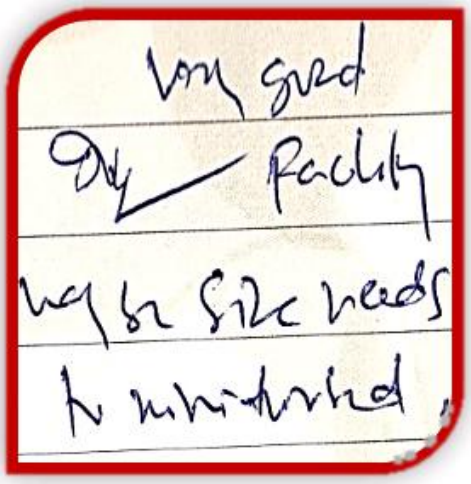

Dr. B. K. Panigrahy, Registrar,
IIIT- Naya Raipur.



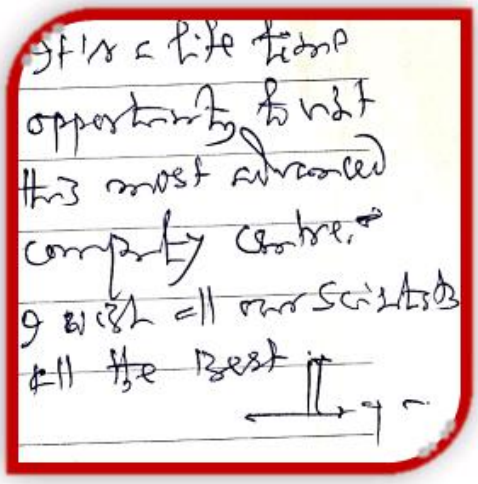

Dr. Pradeep K. Sinha, Vice Chancellor
& Director, IIIT – Naya Raipur.



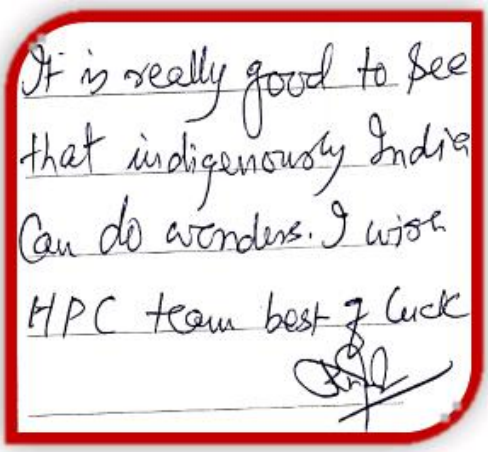

Vice Admiral S. N. Ghormade, AVSM,
Director General, Naval Operations,
Indian Navy.



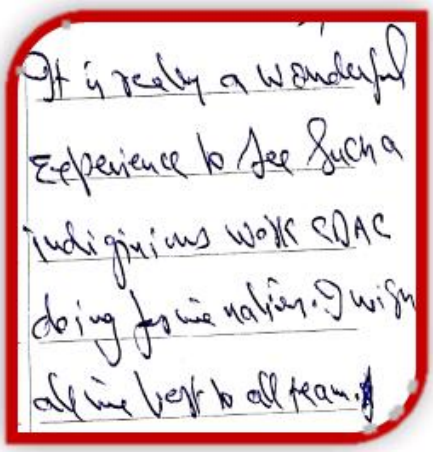

Prof. D. N. Reddy, Director, CR Rao
AIMSCS, HCU, Hyderabad.




Dr. Ajay .K. Nayak, Joint Secretary,
Govt of Odisha, Bhubaneswar.




Prof.R .K. Singh, Dean (Students Welfare), MNNIT, Allahabad.




Shri. M. Krishna, Assistant Director (DOC), CFSL, Hyderabad.


Shri. Jual Oram, Hon'ble Minister of Tribal affairs, Govt of India

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# Appendix F

# Picture Gallery


Visit to NPSF by Shri. Jual Oram ($3^{rd}$ from right ), Hon. Minister of Tribal affairs , Govt of India.


Vinodh Kumar M., Center Head, C-DAC, Mohali & Sr. Director and HoD, HPC-I&E, C-DAC, Pune, explaining about NPSF to Brazilian Delegation.

Visit to NPSF by Brazilian Delegation.


Visit to NPSF by Vice Admiral S N Ghormade ($2^{nd}$ from right ), AVSM, NM, Director General of Navel Operations, Indian Navy.


Visit to NPSF by Dr. Pradeep K. Sinha, Vice Chancellor & Director ,IIIT- Naya Raipur.
[ Dr. Pradeep K. Sinha is the former Senior Director, Corporate R & D, C-DAC. It was under his aegis, NPSF was setup & began offering HPC services to the Nation. ]

Visit to NPSF by Russian Delegation.


Col. A. K. Nath(Retd.), Executive Director, Corporate C-DAC, explaining about NPSF to Lt Gen Anil Kapoor (right), Director General, Information System, Indian Army.

Visit to NPSF by Prof. E .Saibaba Reddy, Former Vice Chancellor, VSSUT, Odisha.

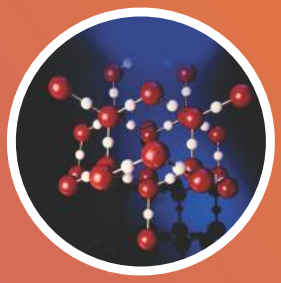

Visit to NPSF by Dr. Ajay K. Nayak, Joint Secretary, Govt of Odisha, Bhubneshwar.

Ms. Nisha Agrawal explaining about NPSF to Media on National Science Day, C-DAC, Pune.

;

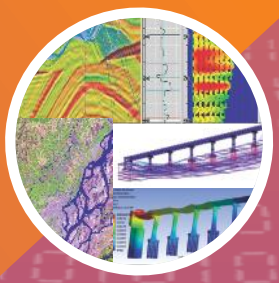



Space Applications



Basic Sciences

Data Sciences



Engineering Applications

Defence & Atomic Energy Applications

Earth Sciences

सी डैक
CDAC
www.cdac.in

प्रगत संगणन विकास केंद्र
CENTRE FOR DEVELOPMENT OF ADVANCED COMPUTING
पुणे विश्वविद्यालय परिसर, गणेशखिंड, पुणे - 411 007, भारत
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