Annual Report

of

National PARAM supercomputing facility

NPSF
National PARAM Supercomputing Facility

2016-17

CENTRE FOR DEVELOPMENT OF ADVANCED COMPUTING

www.cdac.in

Greetings from Director General

Since its inception in 1988, C-DAC has been playing a key role for HPC proliferation in the country. The National PARAM Supercomputing Facility (NPSF) was setup with the purpose of provisioning High Performance Computing (HPC) resources to researchers from various academic and research institutes needing HPC systems for their research. The upgrade of PARAM Yuva to PARAM Yuva II has helped C-DAC to join the Petascale league of Supercomputing centres.

I am privileged to inform that PARAM YUVA II System has completed the processing of 2,25,840 jobs till date and while I am reporting this more jobs are being completed.

Over the years, the NPSF team has gained experience in handling large scale facility and supporting the academic users for their work on PARAM systems. I applaud members of NPSF team for their tireless and unrelenting contribution in supporting to over 940 users from 90 R&D and academic institutions who are using PARAM Yuva II system for their research work. The compute power of the system at NPSF and their user base is expected to increase many fold in the years to come. This report summarizes the activities of NPSF during the year 2016-2017 and showcases the science pursued by the Indian scientific community using this facility. A testimonial of the same is the number of publications in the peer-reviewed National/International journals amounting to 179 and 30 Ph.D thesis submitted by users of the NPSF.

I look forward to their continued commitment in managing a world class computing facility at C-DAC for the ever growing HPC user community in India and in the years to come.

Dr. Debashis Dutta
Director General, C-DAC

Greetings from Executive Director

Since last four years of PARAM Yuva II operations, NPSF has achieved several milestones.The challenge is to cater to the computing needs of ever increasing NPSF user base and the demand for more and more computing power. NPSF adapted a balanced approach in provisioning HPC resources to meet the requirements of both capacity and capability computing.

The usage of the facility above 96% is a clear indication of its effective utilization. This was not possible without the dedicated and quality support offered to the Scientific and Academic community by the NPSF Team. The experience gained by NPSF will certainly help in providing world class services to the HPC user community.

Through National Super Computing Mission (NSM), C-DAC is gearing up to meet the future HPC requirements in INDIA. Under this mission NPSF team contributed in imparting knowledge and training the students of Post Graduate Diploma in High Performance Computing and System Administration (PGDHPCSA) conducted by Advanced Computing Training School (ACTS) towards building HPC Professionals.

I would like to congratulate NPSF user community for their significant achievements leading to 61 publications and 180 students who are pursuing their research work.

Dr. Hemant Darbari
Executive Director, C-DAC, Pune

Greetings from Head of Department

I am very much delighted to put forth the facts and figures of NPSF activities through this Annual Report for the Year 2016-17.

The objective of this report is to present an accurate picture of PARAM Yuva II usage statistics. I believe NPSF put their best efforts in supporting the users and provisioning the resources in a balanced and transparent manner.

PARAM Yuva II utilization of above 96%, study growth in enrolment of new users and projects is a clear indication of NPSF success. I am very much delighted and thankful to the NPSF user community for their faith and confidence in NPSF. I am very sure that NPSF would stand and rise to the user expectations as National Supercomputing Mission(NSM) brings a new era of supercomputing to the nation.

I wish you all Happy Computing.

Mr. Vinodh Kumar M
Associate Director & HoD, HPC-I&E, C-DAC, Pune

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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 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.

PARAM Yuva

The next one in this series was 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 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.

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*.

This report documents the activities of NPSF undertaken during the Year 2016-17.

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Key Highlights

In the Year 2013, increase in the peak compute power from 54 Teraflops to 529.4 Teraflops has been achieved in the same power envelope as that of PARAM Yuva

Facts & Figures

8 February, 2013 PARAM Yuva II dedicated to Nation.

529.4 Tera Flops is the Theoretical peak performance.

386.7 Tera Flops is the Sustained performance.

1,760.20 MFlops per Watt Energy efficiency.

30,056 Computing cores.

221 Computing nodes .

Highlights

2,25,003 Jobs completed processing.

447 Rank as per November, 2016 Top500 list.
[Highest Rank achieved in Top500 supercomputer across globe : 69 in June, 2013 Top500 `http://www.top500.org`]

140 Rank as per November, 2016 Green500 list.
[Highest Rank achieved in Green500 supercomputer across globe : 44 in November, 2013 Green500 `http://www.green500.org`]

940 Users.

90 Institutions.

252 Projects.

30 Completed Ph.Ds.

179 Publications.

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Year 2016 - 2017 in Review

Launched NPSF Scientific User Community Forum (NSCF), socially constructed learning environment for PARAM Yuva II user community

2016

May

With the motive of hosting common platform for NPSF User Community and NPSF System administrators, NPSF Scientific User Community Forum(NSCF) Portal for PARAM Yuva II user community was launched on 23rd May 2016.

June

PARAM Yuva II system has completed processing of two hundred thousand (2, 00,000) jobs on 4th of June 2016.

PARAM Yuva II system was taken into maintenance from 12:00Hrs of 18/06/2016 to 17:05Hrs of 21/06/2016. During the maintenance, following activities were carried out:

- Hardware issue in the HPE StoreAll storage system (PARAM Yuva II home area storage) was resolved
- BIOS upgrade of PARAM Yuva II compute nodes
- Memory issues with NFS Root Servers has been resolved

July

Successfully completed the 3 year collaborative project of SAC (ISRO), Ahmedabad with C-DAC, Pune for execution of their daily operational runs on PARAM Yuva II system on 1024 cores. The success rate of execution of the runs was more than 99% in the 3 years. The project completed on 25th July, 2016.

August

PARAM Yuva II cluster was under maintenance, from 15th August (22:52Hrs) to 18th August (17.30Hrs) due to subsequent failures in Power Supply Subsystem at NPSF.

September	For processing of large number of cores (512 to 1024) jobs with less wall time, a new execution queue BURSTq was introduced on 9th Sept., 2016. The jobs requiring more than 512 and less than 1024 cores for maximum 17:55:00 Hrs wall time jobs were made to route to this queue. Introduction of this queue helped a lot for processing of BIG jobs.
October	Hindi version of PARAM Yuva II Annual Report for FY:2015-2016 was released by C-DAC Pune Executive Director Dr. Hemant Darbari on 14th Oct 2016 on the occasion of Hindi Diwas. Hindi version report of PARAM Yuva II was prepared by NPSF Team solely using C-DAClanguage processing tools. PARAM Yuva II cluster was partially not available from 9th Oct16(17:19Hrs) to 10th Oct16(18:07Hrs) due to power failure in Power Supply Subsystem at NPSF.
November -December	NPSF team members have delivered the lectures and conducted the Lab sessions related to HPC system Administration for the students of PG-DHPSA (Post Graduate Diploma in HPC System Administration) course, run by Advanced Computing Training School (ACTS), C-DAC, Pune.
2017	
January	On January 27, 2017, Ms. Nisha Agrawal delivered invited talk on Introduction to OpenCL Computing for faculties and students of Pune Institute of Computer Technology (PICT), Pune.
February	As a part of National Science Day celebration at C-DAC on February 28, 2017, NPSF team participated in the event and showcased the activities related to PARAM Yuva II. Around 1500 visitors (Students from various colleges and schools) from Pune and nearby districts like Mumbai enjoyed the technical sessions and walk-through of PARAM Yuva-II.
March	Provided PARAM Yuva II computing resources support for International High Performance Computing (IHPC) competition as part of Techkriti 17 organized by IIT, Kanpur between March 23-26,2017. On March 11, 2017, Mr. Y. S. Swarup delivered invited talk on "Setup and handling of IT infrastructure in DC" during One Week Short Term Training Programme on "Network System Administration and Security (NSAS)" at College of Engineering Pune (COEP).

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PARAM Yuva II Insights

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

Intel Xeon Phi 5110P with 60 cores such two accelerator cards per compute node

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

Four subclusters	
Subcluster 1	221 nodes cluster of Intel server system R2000GZ with Dual socket Intel Xeon E5 2670 (Sandy Bridge) Processor per node Eight CPU cores per socket, 2.6 GHz Two Intel Xeon Phi 5110P per node Infiniband FDR interconnect Partitions: TESTp, FDRp, BIGJOBp, MICp, SDSp
Subcluster 2	60+ nodes cluster of HP Proliant DL580 G5 with Quad socket Intel Xeon X7350 Processor per node Four CPU cores per socket, 2.93 GHz System interconnects: PARAMNet3, Infiniband DDR Partition: DDRp
Subcluster 3	Four nodes cluster of Supermicro SuperServer 1027GR-TRF with Dual socket Intel Xeon E5 2650 (Sandy Bridge) Processor per node Eight CPU cores per socket, 2.6 GHz Two NVIDIA GPU Tesla M2090 per node Infiniband FDR interconnect Partition: GPUp

Subcluster 4	Supermicro 4U AMD SR5690 SMP server with 64 cores Quad socket AMD Opteron 6276 Processor Sixteen CPU cores per socket, 2.3 GHz 512 GBytes of RAM Partition: (grouped with) GPUp
Storage	HPC Scratch area with 10 GB/s write bandwidth over Parallel File System Reliable User Home Area: 100TB Backup: 400TB (native capacity)
Software	Operating System: CentOS v6.2, Kernel v2.6.32-220 Intel Cluster Studio XE 2013 Intel Cluster Studio XE 2015 PGI Cluster Development Kit
Applications	Libraries and software for file formats, data bases and math Many scientific applications for material science/quantum chemistry, molecular modelling, fluid dynamics, climate modelling and circuit simulations and many more like aerospace engineering.

The cluster partitions have been created in order to improve the quality of service.

Partitions and Queues:

Resources on PARAM Yuva II are grouped into homogeneous groups known as partitions. Table-4.2 shows the summary of partitions and their mapping to job submission queues.

Table 4.2: Summary of queues and partitions on PARAM Yuva II

Partitions	Queue	Wall Time Limit	Accelerator(s) in the nodes in the partition
FDRp	batch	7 Days	Xeon Phi
BIGJOBp	batch	7 Days	Xeon Phi
TESTp	TESTq	2 Hours	Xeon Phi
GPUp	GPUq *	7 Days	GPU
MICp	MICq	7 Days	Xeon Phi
SDSp§	SDSq †	06 Hours ‡	Xeon Phi
SDSp	BURSTq ¶	17 Hours 55 Minutes	Xeon Phi

Various queues ensures a spectrum of quality of service according to the resource requirement of the users for different computing exercises.

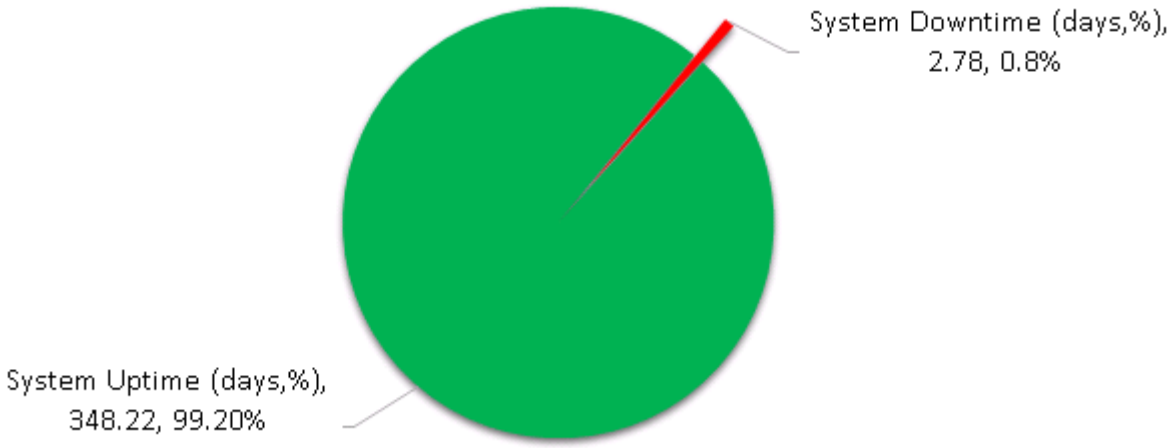
- With the availability of TESTp partition, the users get resources without having to wait longer to run the test jobs before the actual job runs. Currently the maximum allowed walltime for TESTq queue is 2 Hrs per job.

- The queue wait time for the jobs with resource request of more than 64 cores has been reduced considerably with the availability of BIGJOBp partition

- The resources in the SDSp partition are primarily for running the production jobs on daily basis for a fixed duration as per the commitment to different users. The resources in this partition during their idle time have been made available to jobs requiring large number of cores for less walltime, thus reduce the wait time for larger jobs. (BURSTq).

*Queue for jobs with GPU nodes/SMP node.
†Queue for jobs on resources with advanced reservation.
‡Idle period of the committed resources (on daily basis for 7 consecutive days).
§Partition with committed resources for production jobs.
¶Queue for jobs requiring large number of cores for less wall time.

PARAM Yuva II availability: (Period: Apr. 1, 2016 - Mar. 15, 2017) [351 Days]



- Uptime: 348.22 Days
- Maintenance Period: 2.78 Days
  - August 15,2016, 10:53 PM to August 18,2016, 05:40 PM [2 Days, 18 Hrs, 47 Minutes]
- System uptime: **99.20%**

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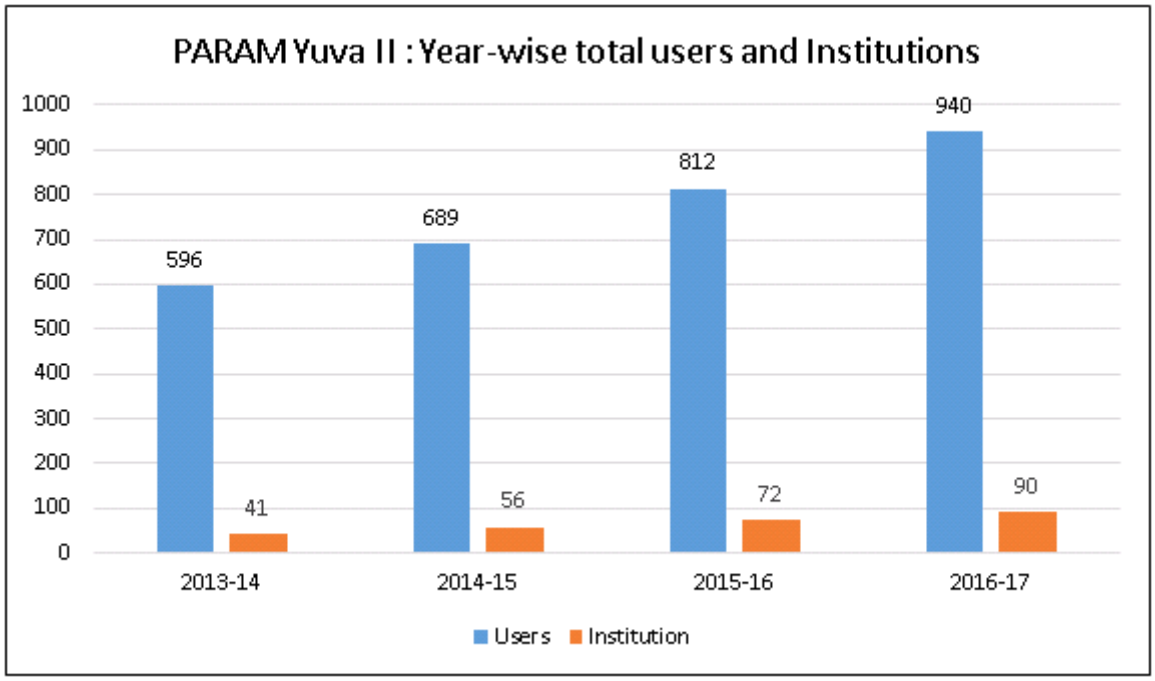
Users and Usage Statistics

In Year 2016-17 : Users added : 112 ; Institution added : 17 ; Jobs Processed : 32,232

Projects & Users (as of 15^{th} March 2017)

- Number of projects : 252
- Number of users: 940 (across 90 Institutions)
- Number of PhD students: 188



Users across Institutions

Table 5.1: 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
BITS Pilani, Hyderabad Campus	2
CMR College of Engg. & Tech.	2
Carnegie Mellon University	1
College of Engineering, Pune	2
Central Univ. of Bihar	1
Central Univ. of Gujarat	3
Central University of Haryana	3
Delhi University	2
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
Himachal Pradesh University	3
IIA, Bangalore	12
IIIT, Hyderabad	3
IIIT, Delhi	4
IISc, Bangalore	7
IISER, Pune	52
IISER, Mohali	1
IISER, Thiruvananthapuram	3
IIT Bombay	204
IIT Bhubaneswar	2
IIT Delhi	8
IIT(ISM) Dhanbad	2
IIT Guwahati	23
IIT Gandhinagar	10
IIT Hyderabad	26
IIT Jodhpur	10
IIT Kanpur	23
IIT Kharagpur	12
IIT Patna	7
IIT Ropar	8
INST, Mohali	14
JMI University	1
Jiwaji University	3
JNU	2

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Table 5.1 – *Continued from previous page*

Academic Institutions	No. of Users
Kurukshetra University	3
Manipal University	2
MIT Pune	1
NIT Calicut	1
NIT Rourkela	1
Panjab University	2
PJTSAU, Hyderabad	1
PDU Shekhawati Univ., Sikar	1
PU College, Mizoram	1
RTM Nagpur University	2
SASTRA University, Thanjavur	3
Shekhawat University	1
SRM University	3
SRTM University	2
St. Xavier's College, Ahmedabad	1
S P Pune University	36
Sri Guru Granth Sahib World University	4
Tejpal University	1
University of Hyderabad	1
University of Rajasthan	1
VNIT Nagpur	10
Total	**559**

Table 5.2: Users across research institutions

Research Institutions	No. of Users
BARC, Mumbai	1
CBS, Mumbai	2
CIFRI, Kolkata	2
C-DAC	137
CECRI, Karaikudi	4
DRDO-BU Centre for Life Sciences, Coimbatore	4
E-teacher	2
GARUDA	165
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	10
NABI, Mohali	1
NCL, Pune	6
NCRA, Pune	6
NIC	2

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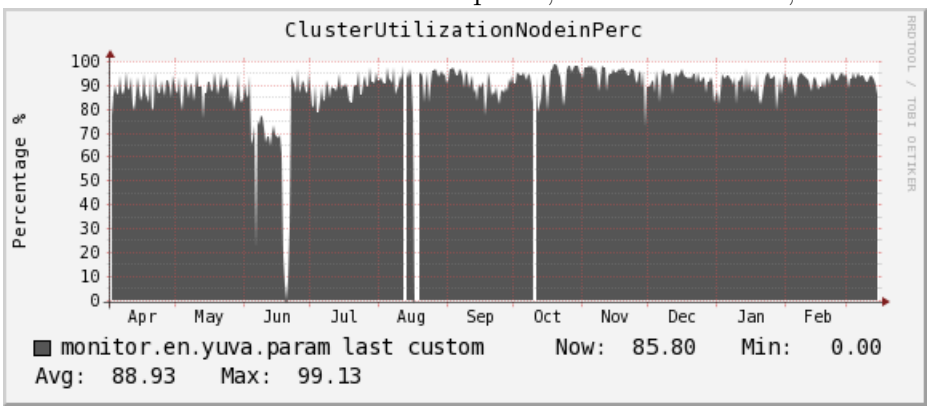
Table 5.2 – *Continued from previous page*

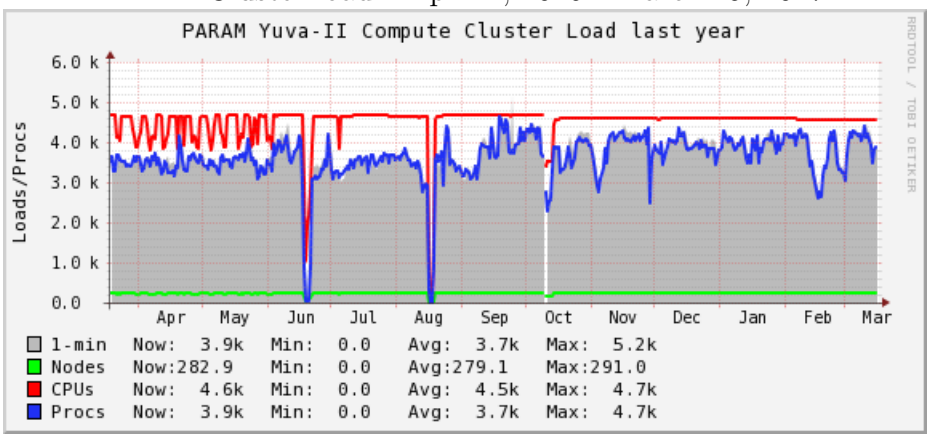
Research Institutions	No. of Users
NISER	1
PRL, Ahmedabad	3
RRI, Bangalore	3
SINP, Kolkata	2
THSTI	4
Vijay Kumar Foundation, Gurgaon	6
Total	**381**

PARAM Yuva II System utilization:

Cluster Utilization : April 1, 2016 - March 15, 2017



Cluster load : April 1, 2016 - March 15, 2017



The maintenance activity of PARAM Yuva II accounts for the gaps in the months of May (from 12:00Hrs of 18/06/2016 to 17:05Hrs of 21/06/2016) and August (from 22:52Hrs of 15/08/2016 to 17.30Hrs of 18/08/2016) in the utilization graph (top).

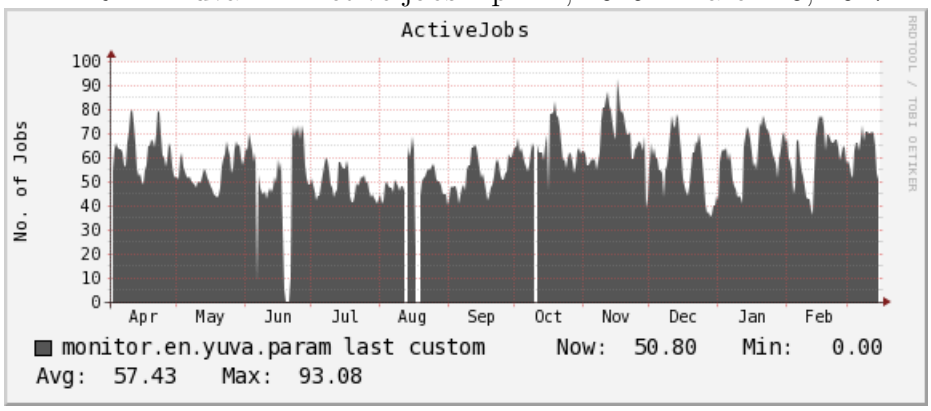
There was a partial shutdown of PARAM Yuva II (some of the nodes) in the month of October (from 17:19Hrs of 09/10/2016 to 18:07Hrs of 10/10/2016) due to issues

related to power and cooling infrastructure. The partial shutdown during this period, is reflected in the depletion of CPU cores from the complementary data from Ganglia (bottom).

Job Queues:

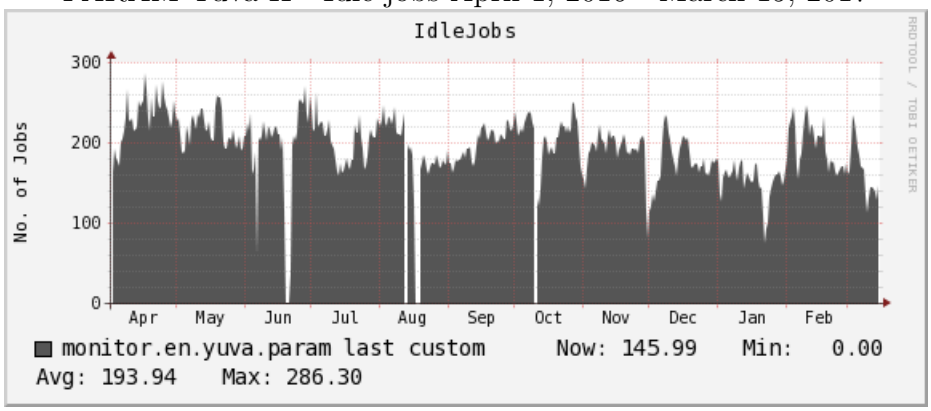
Running Jobs (Active Jobs)

PARAM Yuva II - Active jobs April 1, 2016 - March 15, 2017



Idle Jobs (Jobs waiting in queue for execution)

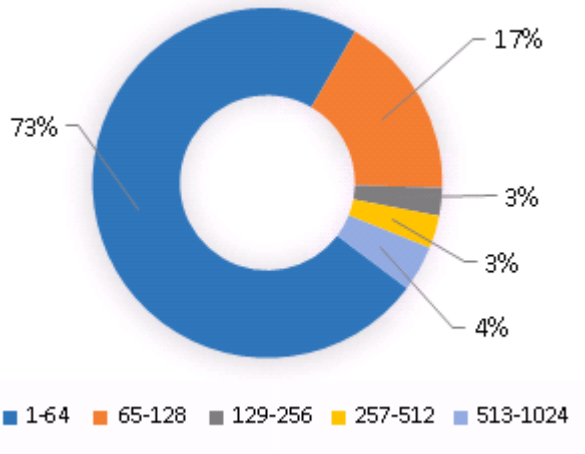
PARAM Yuva II - Idle jobs April 1, 2016 - March 15, 2017



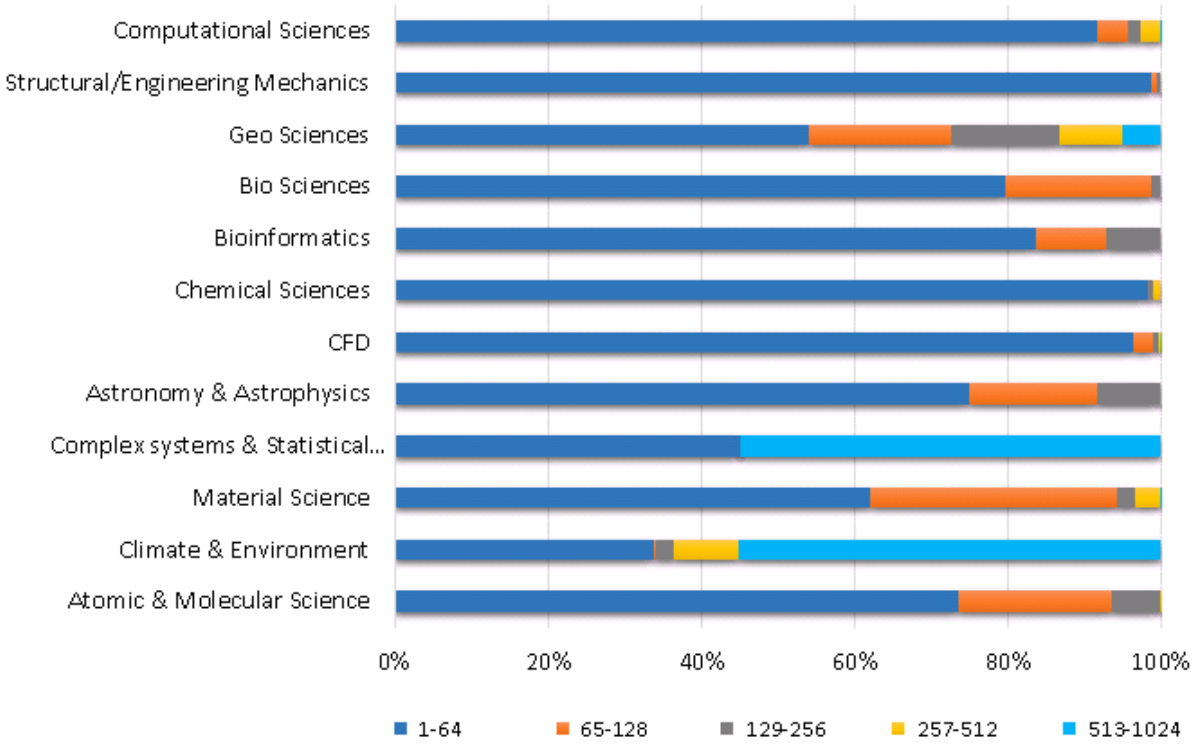
From the figures above, we see that about 57 jobs are running on an average and 3 times more number of jobs are always in queue waiting for their turn to start running. This indicates the need for more resources.

CPU Utilization (Period: April 1, 2016 - March 15, 2017)

CPU Time utilization vs no. of cores

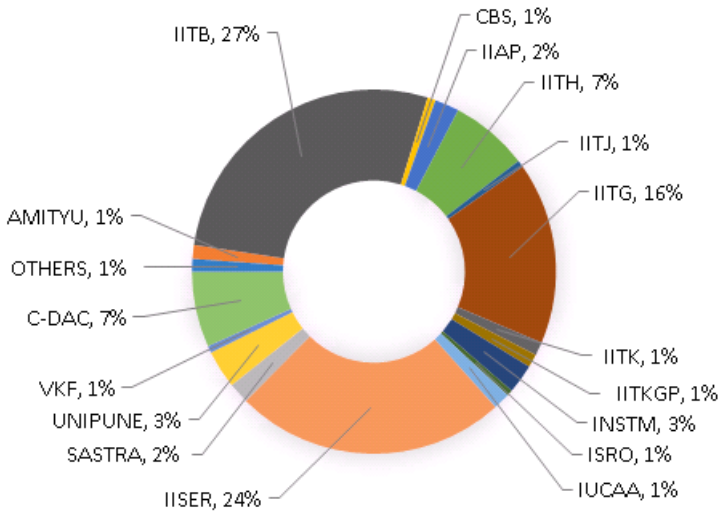


Job Size (CPU cores) across application domains

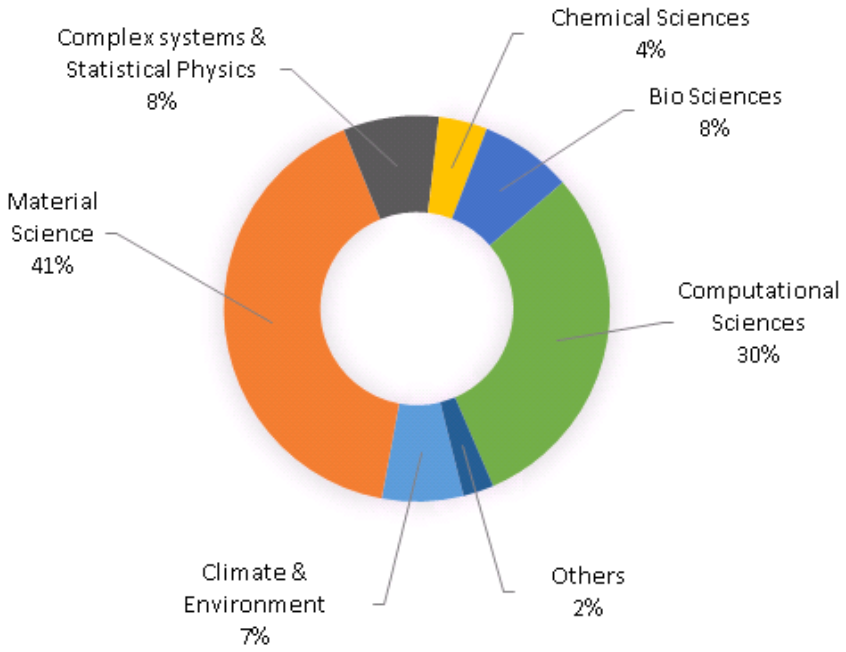


CPU Utilization (Period: April 1, 2016 - March 15, 2017)

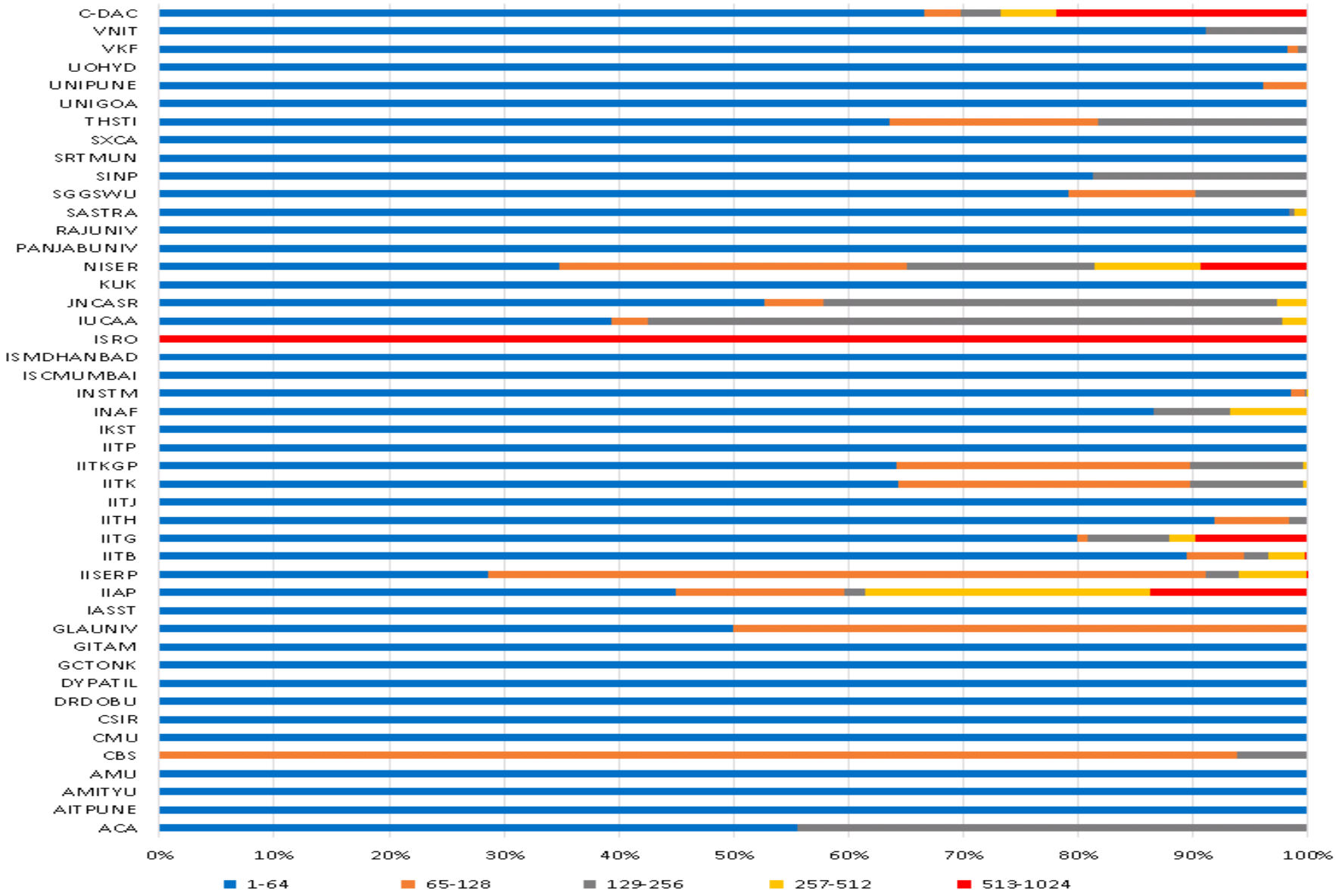
Institute wise CPU utilization (in %)



CPU time utilization (in %) across application domains

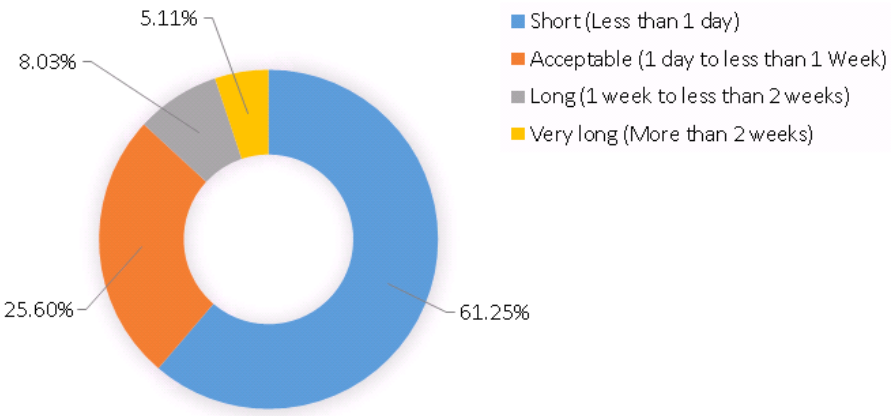


Job Statistics (Period: April 1, 2016 - March 15, 2017)



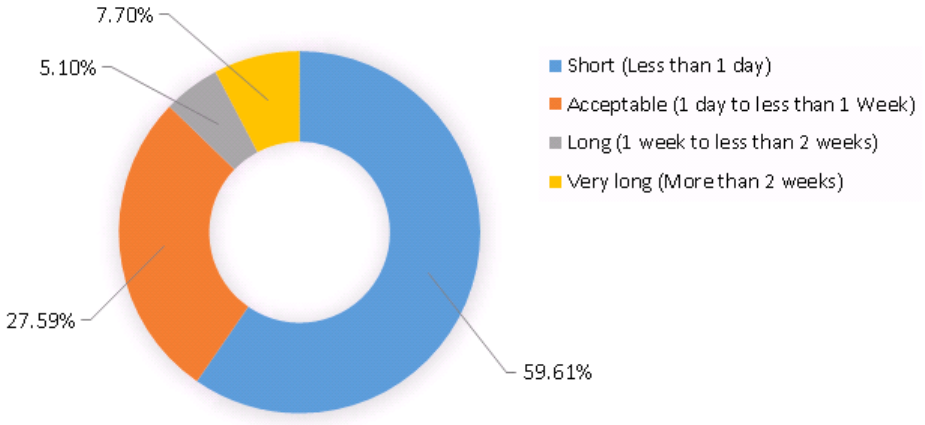
Job Statistics (Period: April 1, 2016 - March 15, 2017)

Queuetime for small jobs (Jobs requiring less than 65 cores)



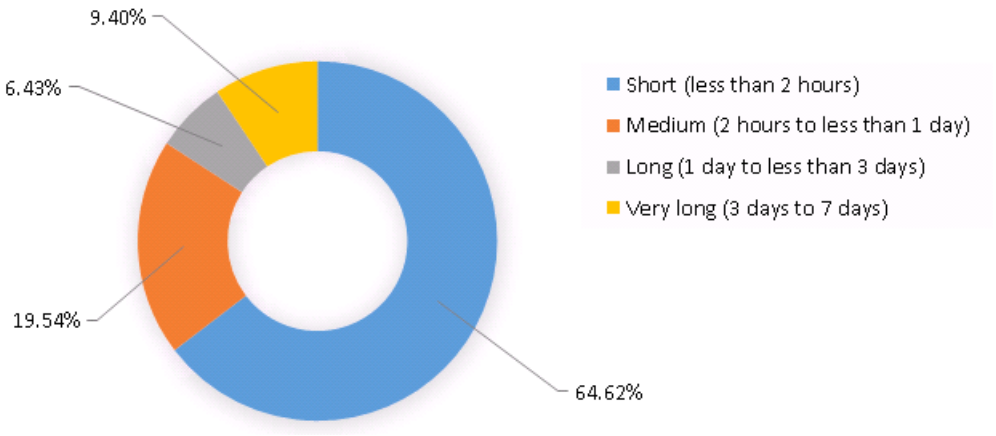
Above graph shows the queue time (time spent by the job in the queue before going for execution) analysis of the small jobs (jobs requiring less than 65 cores). It is observed that the more than 60% of the small jobs gets executed spending less than 1 day in queue.

Queuetime for big jobs (Jobs requiring greater than 64 cores)



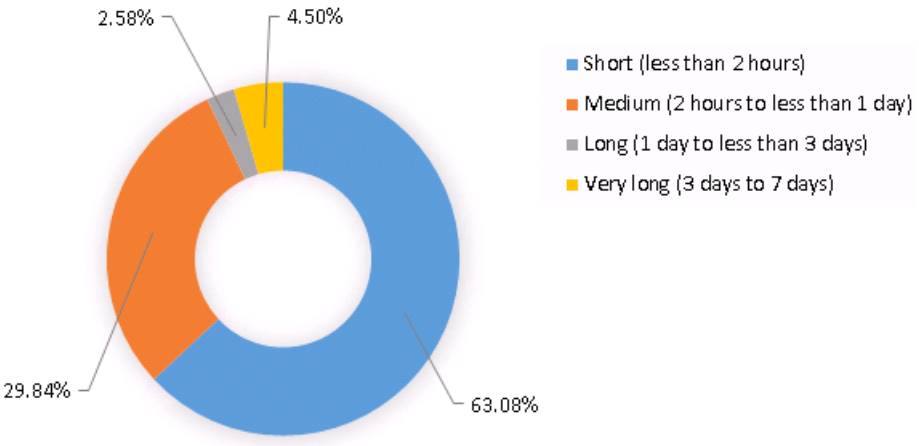
Above graph shows the queue time (time spent by the job in the queue before going for execution) analysis of the big jobs (Jobs requiring greater than 64 cores). It is observed that about 60% of the big jobs gets executed spending less than 1 day in queue.

Execution time for small jobs (Jobs requiring less than 65 cores)



Above graph shows the execution time (Runtime of job) analysis of the small jobs (jobs requiring less than 65 cores). It is observed that about 65% of the small jobs gets executed within 2 hours of time. The data is irrespective of exist status of jobs.

Execution time for big jobs (Jobs requiring greater than 64 cores)



Above graph shows the execution time (Runtime of job) analysis of the big jobs (Jobs requiring greater than 64 cores). It is observed that about 63% of the big jobs gets executed less than 2 hours of time. The data is irrespective of exist status of jobs.

Jobs statistics:

Number of Jobs = 32,232 (Period: April 1, 2016 - March 15, 2017)

Total Number of Jobs = 2,25,003 (Period: February 19, 2013 - March 15, 2017)

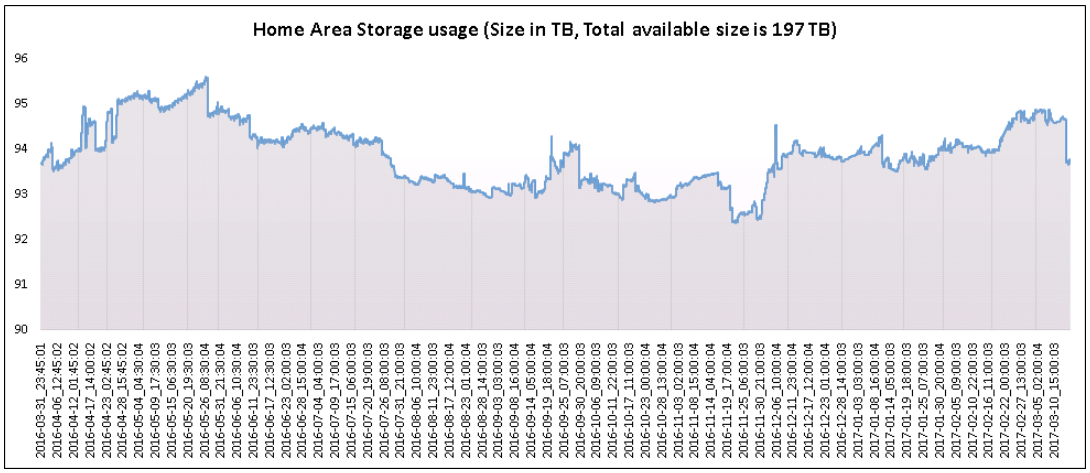
Jobs across Domains

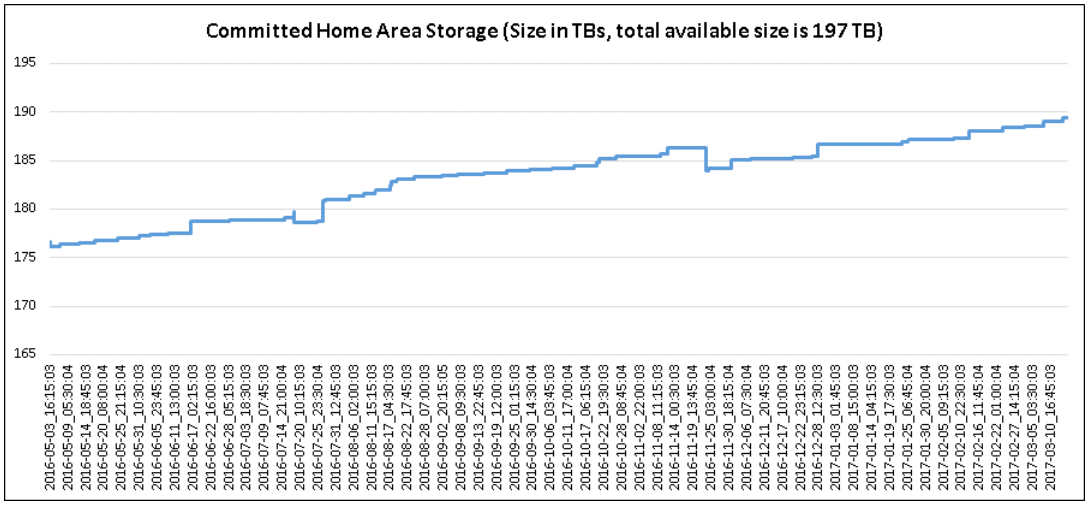
Table 5.3: Jobs across Domains

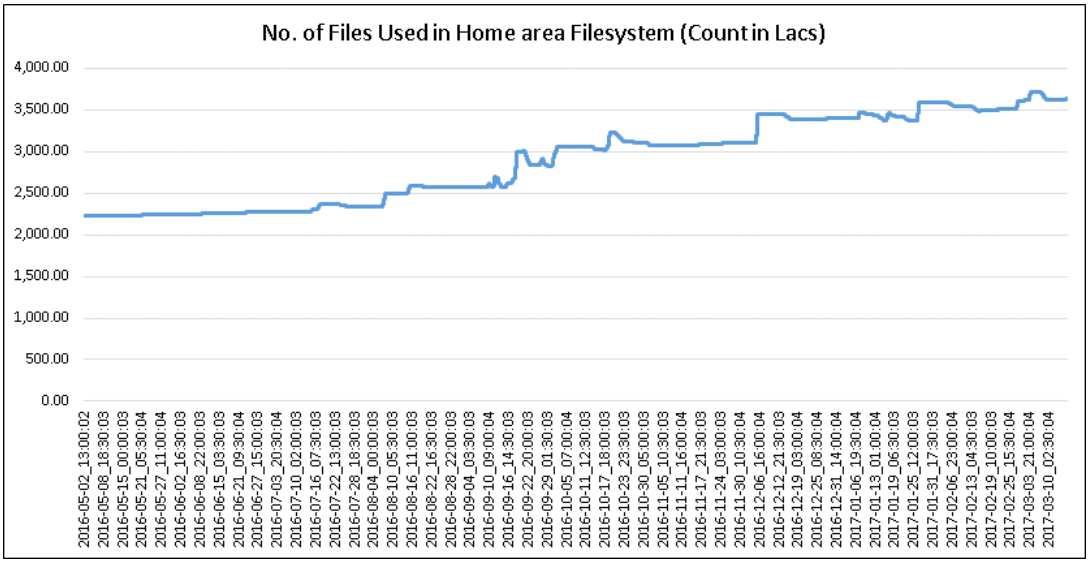
Domain	Jobs
Atomic & Molecular Science	1570
Climate & Environment	2135
Material Science	13556
Complex systems & Statistical Physics	219
Astronomy & Astrophysics	12
CFD	480
Chemical Sciences	2333
Bio Informatics	140
Bio Sciences	1033
Geo Sciences	554
Structural/Engineering Mechanics	758
Computational Sciences	9442
Total	32232

Storage usage statistics:

The statistics of the PARAM Yuva II home area occupancy, committed home area and number of files used in home area, are shown in the plots below.

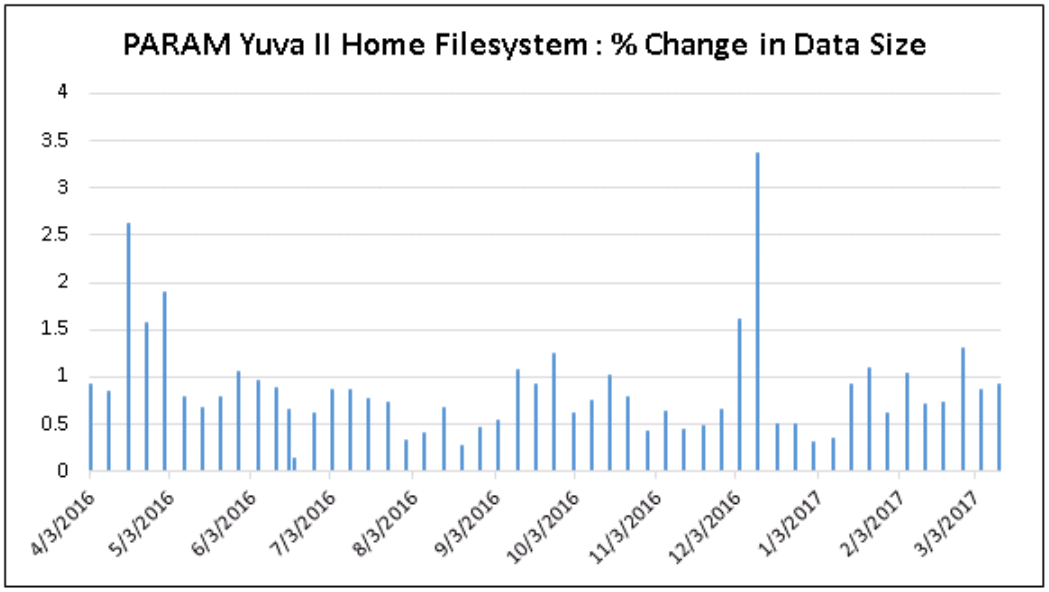


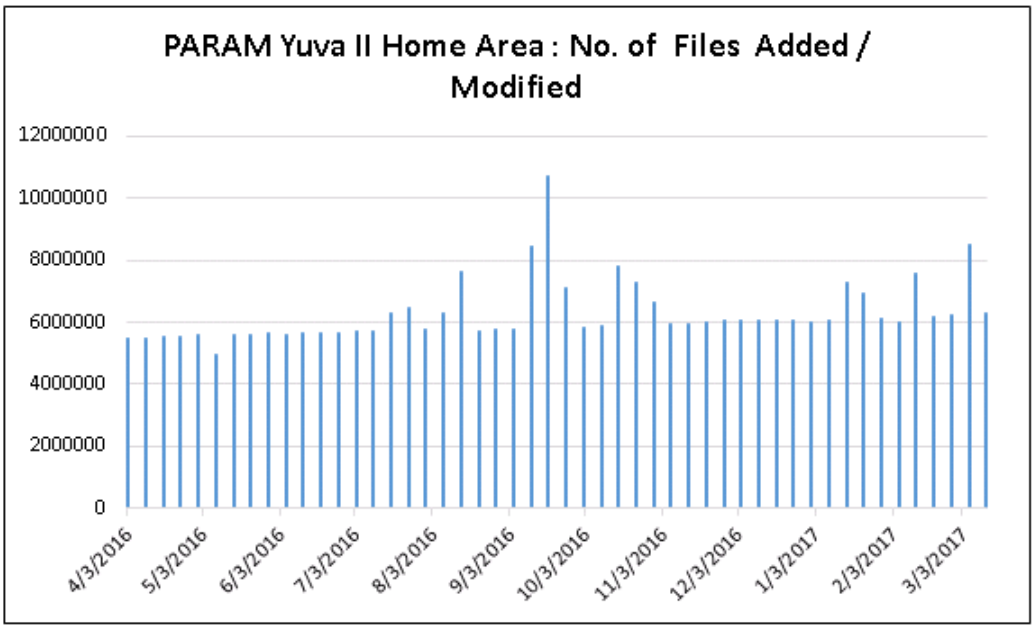




Every user of PARAM YuvaII has a storage quota allocated. Total of such quota allocations is above 96 % of the available storage space. The committed home area increased from 89.51 % to 96.14% in last 1 Year of time.This is an indicator for the requirement of expansion of the storage. The activity has been planned in the coming year.

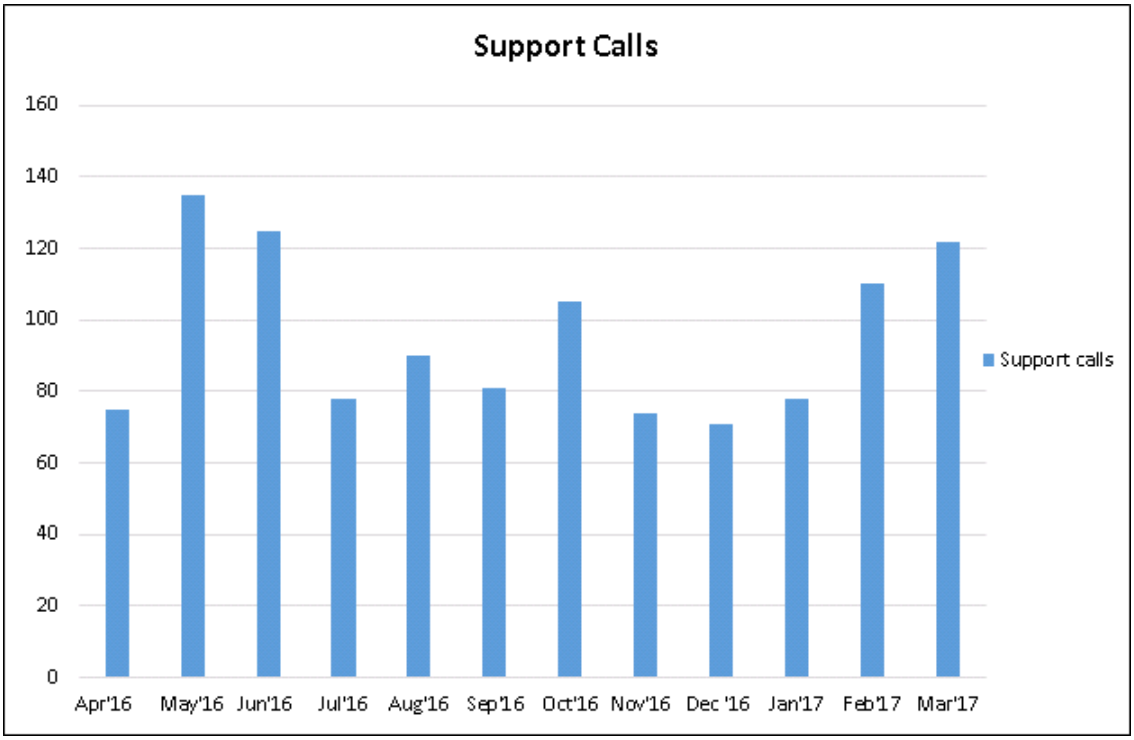
Besides the default quota allocations, an additional quota is allocated to user as per the request for fixed short durations. The storage is divided into home area and high performance scratch area as mentioned in the compute resources.





User Support Calls:

The NPSF-Help team handles about 95 user support calls every month. The statistics for the last one year is shown below. The mode of extending the support to the users include, telephonic support, shared screen sessions, e-mail and at times visits by the users. The data used for this statistics are the ones primarily gathered through the e-mail support calls.


Support Calls
160
140
120
100
80
60
40
20
0
Apr'16
May'16
Jun'16
Jul'16
Aug'16
Sep'16
Oct'16
Nov'16
Dec '16
Jan'17
Feb'17
Mar'17
Support calls

6

Publication Reports

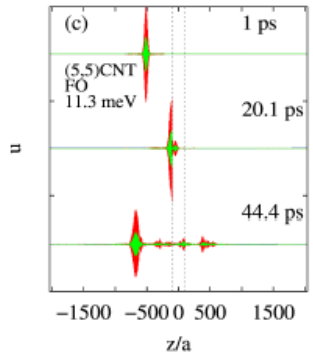
Some of the publication reports based on the research publication/s in high impact journals from the work that has been carried out on PARAM Yuva II.

Phonon Scattering Dynamics of Sliding Motion in Carbon Nanotube Oscillators

CI: Dr. Baidurya Bhattacharya
baidurya@civil.iitkgp.ernet.in

INSTITUTION: IIT Kharagpur

RESEARCH DOMAIN: Material Science



FO phonon with 11.3 meV interacting with (5,5) CNT-L50.|

Research Challenge

Several theoretical and experimental attempts have been made to explore the thermophoretically driven transport of molecular structures. Attaining controlled motion in nanoscale has been a challenging task, thermophoresisthermal gradient induced forceis one of the popular driving mechanism of molecular systems. The essential driver for such motions is the net current of hot phonons that are generated by the imposed thermal gradients. While interacting, these hot phonons are scattered by the moving object and some of the vibrational energy is exchanged with translational energy of the moving body. However, there have been few attempts to gain phonon level understanding of thermophoretic motion, and the exact underlying physical mechanism has remained elusive so far.

The challenge is to understand the fundamental mechanism of how individual phonons interact with the moving molecular system and how phonon characteristics influence the sliding process. Further, at the initiation of sliding process, how the phonon could able to push the molecular system over its potential barrier is extremely curious.

Approach

Under quasi-particles treatment, phonons can be modeled as wave packets by attributing position and momentum. However, for a typical wave length of the phonon, it spans over few hundreds of nanometers. Thus, our system of double walled CNT oscillator consists of (10,10)CNT of 1000 nm long as outer casing and (5,5)CNT of 50-200 nm long as inner sliding nanotube. Molecular dynamics of such a micron long system demands an expensive computational resources.

In this approach, a phonon wave packet with polarization, s, and wave number, q0, at location, z0, is constructed from the linear combination of vibrational eigen modes of the lattice according to

$$u^{s}_{lk\alpha} = \frac{A}{\sqrt{M}} \sum_{q} \exp\left[\frac{(q-q0)^2}{2\sigma^2}\right] e^{s}_{k\alpha}(q) \exp\left[iq(z_l - z_0)\right]$$

where $u^{s}_{lk\alpha}$ is the displacement from the ground state position of the k^{th} base atom in the l^{th} unit cell (located at z_l) along direction α. A is the amplitude of the wave packet, and M is the mass of the atom. $e^{s}_{k\alpha}(q)$ is the phonon eigenvector corresponding to polarization, s, and wave number, q. σ is the broadening parameter in the Gaussian spread of the wave packet around q0. The eigenvectors, $e^{s}_{k\alpha}(q)$, and corresponding phonon frequencies ω^s (q) are obtained by diagonalizing the dynamical matrix which is the Fourier transform of the force constant matrix. The phonon frequency vs. wave vector plot gives the dispersion relation $\omega^s(q)$.

A wave packet is generated in the outer tube far away from the inner core (500 unit cells to the left of the centre, with $= 2/100a$ (where a is the lattice constant) giving a spread of 200 unit cells) and we study how the individual phonon travels through the outer CNT, interacts with the inner nanostructure, and generates a net driving force. Molecular dynamics simulations are conducted in microcanonical ensemble with a time step of 1 fs using LAMMPS. By repeating such imposition of wave packets of frequencies covering the entire spectrum of for a particular polarization, evaluate the energy transmission coefficient (the ratio of transmitted energy to the incident phonon wave packet energy) for all frequencies results the phonon transmission function.

Results

A through presentation of the results can be found in PhD thesis [M. V. D. Prasad, Phonon Scattering Dynamics of Sliding Motion in Carbon Nanotube Oscillators, PhD thesis, Indian Institute of Technology, Kharagpur, 2016] and in our publication [NanoLett, 16, 2174(2016)].

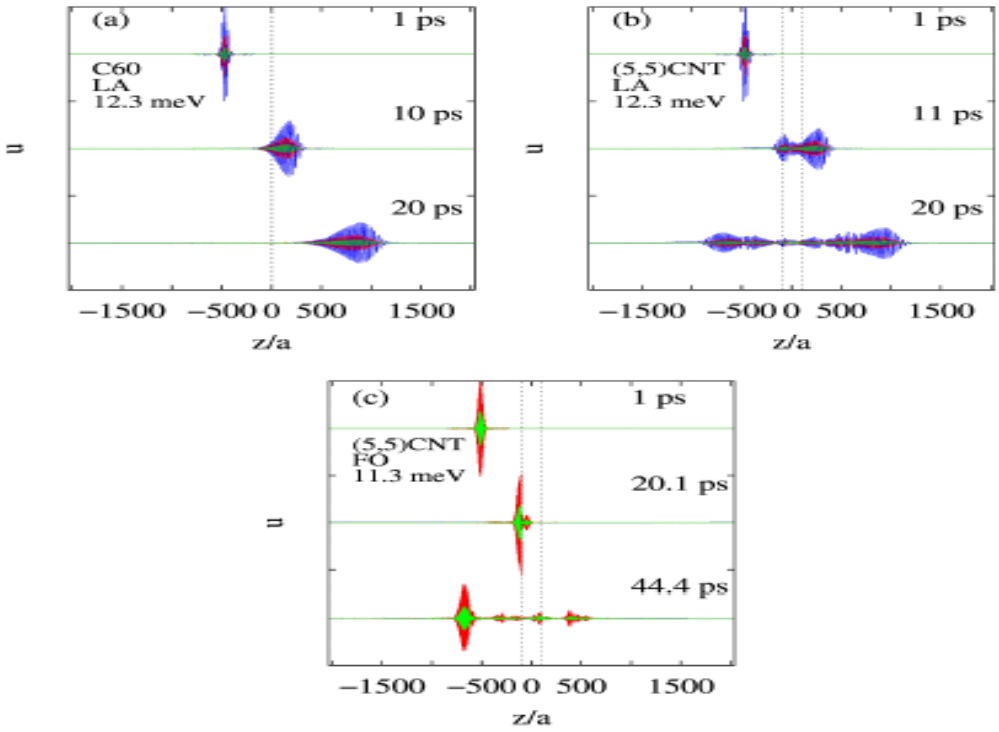


Figure : Wave packet propagation. Snapshots of the displacements for wave packets before, during and after interface scattering. LA phonon with (a) 5.76 meV interacting with a C60 (b)12.3 meV interacting with (5,5) CNT-L50 and (c) FO phonon with 11.3 meV interacting with (5,5) CNT-L50. Vertical dashed lines indicate the position of inner CNT. The axial and two transverse components of wave packet displacement are represented in blue, green and red respectively.

Impact

By showing that thermophoretic motion in coaxial CNTs is initiated by LA phonon scattering mechanism, this work builds a connection between phonon scattering dynamics and nanoscale mechanical motion. We have shown that the scattering mechanism of LA mode phonons, particularly in low to moderate energy ranges, generates a net axial force on the encapsulated nanotube. The length dependence of thermophoresis is elucidated by LA mode transmission functions.

The knowledge of precise interaction mechanism of individual phonons with the inner nanostructure would lead to nanoscale motion control in nanomechanical and biotechnological applications.

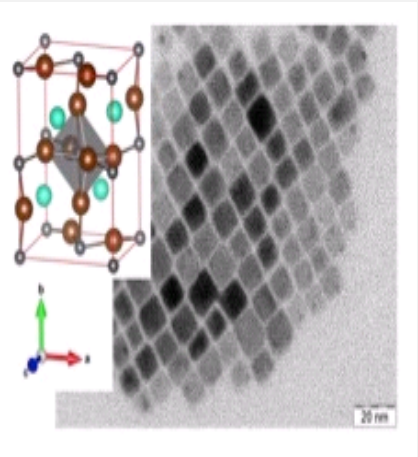
How this research work is benefited using PARAM Yuva II

Simulation of micron long atomic systems for few hundreds of nanoseconds using LAMMPS is not feasible without PARAM facility. To compute one transmission function, around 20-30 cases with wave packets at different frequencies need to be simulated each involves an expensive computational load. We have computed several such transmission functions. In total, it is a computationally demanding task and we did it with the help of PARAM YUVA II.

Experiences using PARAM Yuva II (system, support etc.)

Importantly, every time when we approached npsfhelp@cdac.in, the support is very prompt and encouraging. Over the years, we observed enhanced speed of computations and, of course, the increased number of users. At present, it is exceptionally fast. Overall availability of nodes and wall time is very much satisfactory.

THz conductivity within colloidal CsPbBr3 perovskite nanocrystals: remarkably high carrier mobilities and large diffusion lengths



CI: Dr. Prasenjit Ghosh
pghosh@iiserpune.ac.in

INSTITUTION: IISER Pune

RESEARCH DOMAIN: Material Science

Research Challenge

To investigate the carrier mobility and their diffusion lengths in CsPbBr3 perovskite and to understand the origin of the excellent photo perovskite and to understand the origin of the excellent light emitting properties.

Approach

To achieve the above mentioned challenges we used a combination of pump-probe THz experiments and first principles calculations.

Results

The ground state properties (structural and vibrational) were characterized by Transmission electron microscopy, THz time domain spectroscopy and DFT calculations. These are summarized in Fig. 1.

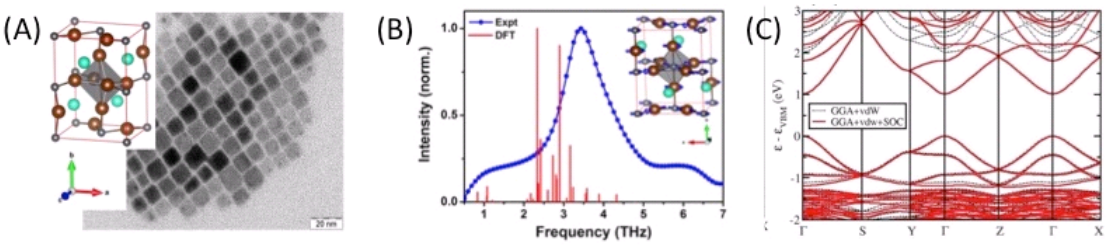


Figure 1. (A) TEM image of synthesized CsPbBr3 NCs. The inset shows the bulk orthorhombic crystal structure as obtained from the DFT calculations, (B) Normalized THz-TDS absorption spectrum (blue solid circles) of NCs and optical phonon intensities (red sticks) from DFT calculation, and (C) the band structure of bulk CsPbBr3 with and without SOC.

From our calculations we estimated the exciton binding energy. Our calculations predict that depending on the value of the dielectric constant, the exciton binding energies

can vary between 6.0 meV to 90.0 meV. Further we also found that the effective masses of the holes and electrons in this material are similar and is about 0.25. These along with the THz pump-probe experimental data were used to estimate the intrinsic carrier properties in this material. We find that the electron and hole carrier mobilities are about 4500 $cm^2V^{-1}s^{-1}$ while their diffusion lengths are greater than 9.2 To put our results in proper perspective, we have compared the above mentioned properties with that of other semiconducting nanocrystals and single crystals. These are given in Table 1. We find that for CsPbBr3 these values are orders of magnitude higher compared to those found in the hybrid halide perovskite films and comparable to single crystalline bulk semiconductors. These values will certainly reduce in a device configuration, but are anticipated to remain much higher compared to other semiconductor NCs. Therefore, CsPbBr3 NCs are promising candidates for applications in optoelectronic and photovoltaic devices.

Table 1. Comparison of mobility and diffusion length of CsPbBr3 NCs with those of other important NCs and single crystals.

Material	Mobility ($cm^2V^{-1}s^{-1}$)		Diffusion Length (μm)		Measurement technique
	Electron	Hole	Electron	Hole	
$CsPbBr_3$ NC (this work)	~4500	~4500	≥ 9.2	≥ 9.2	THz
$CsPbBr_3$ single crystal[64]	~1000				PC
$MAPbBr_3$ polycrystalline film[5]	30		0.3 – 1		THz
$MAPbBr_3$ single crystal[10]	~115	20-60	3 - 17		TOF/Hall/TA/TRPL
$MAPbI_3$ single crystal[69]	500-800	500-800			THz
CdSe NCs[42]	~1-100				THz
CdSe bulk[42]	~470	~145			THz
GaAs crystal[70]	~8000	~400	7	1.6	Hall
Si crystal[70]	~1450	~500	1000	600	Hall
PbTe crystal[70]	~6000	~4000			Hall

MA = CH_3NH_3, THz = terahertz spectroscopy, PC = photoconductivity, TOF = time of flight, TA = transient absorption, TRPL = time resolved photoluminescence

Impact

To the best of our knowledge this is the first study to quantify the intrinsic properties of the charge carriers in this material. We show that the excitons in this material are weakly bound and hence easy to dissociate. Additionally the defect states are not optically active. All these combined give rise to excellent light emitting properties.

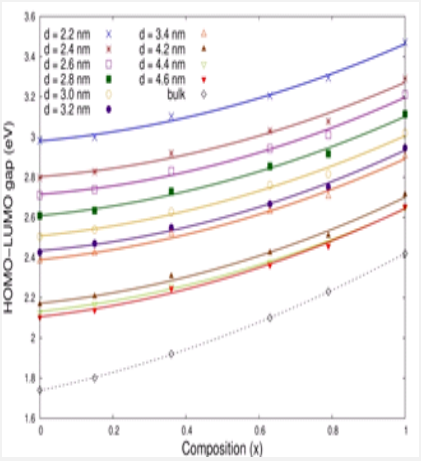
How this research work is benefited using PARAM Yuva II

Performing DFT calculations with spin orbit coupling interactions included are expensive. Having access to PARAM Yuva II made these calculations possible.

Experiences using PARAM Yuva II (system, support etc.)

The system and support is excellent. However, the waiting time for jobs is enormously large. Hence when working with novel and interesting materials where one needs to compete with large groups abroad, this becomes a detrimental factor.

Effect of substitutional doping on electronic structure of II-VI semiconductor quantum dots.



CI: Prof. Anjali Kshirsagar
anjali@cms.unipune.ac.in

INSTITUTION: Savitribai Phule Pune Univ.

RESEARCH DOMAIN: Material Science

Research Challenge

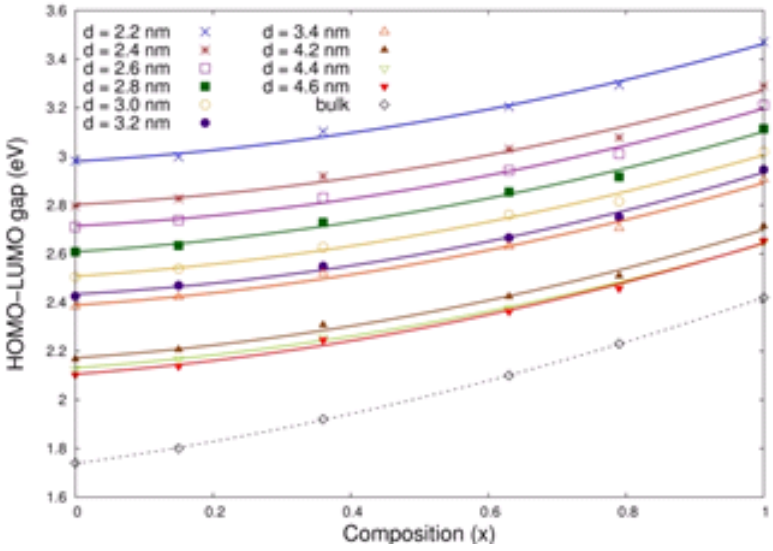
Materials, in particular, semiconductors, are found to change most of their electronic properties and related parameters at nano scale even though they show crystal structure similar to their bulk counter parts. When the size of the nanoparticles or quantum dots as they are normally termed, is comparable to the Bohr exciton radius of the bulk semiconductor, normally the size is of the order of few angstroms, the change in electronic properties is dramatic. To simulate the properties at nanoscale, we need to arrange few hundreds to few thousands of atoms (depending on size of quantum dots) in periodic order defined by their bulk structure. Challenging task is to obtain the minimum energy geometry called optimized structure for particular size to get accurate simulated electronic properties of quantum dots. Such time consuming and memory intensive computation is too difficult to be carried out on available machines.

Approach

We have used VASP package to obtain all our results. We tackle the challenging task by using parameters observed experimentally such as crystal structure, size, shape, element content i.e. doping value of quantum dots. We have used passivating atoms to satisfy the dangling bonds on the surface of the quantum dots and have not carried out geometric relaxation. We have confirmed that passivation locks the symmetry and therefore there is no need to minimize the total energy. Since parameters were experimentally observed results obtained are comparable to experiments and hence the reality. In this way we are able to generate reliable results with the available computing facility at C-DAC, Pune. In addition to the size of quantum dots, alloying provides another to vary the electronic properties. At nanoscale, sometimes, it is desirable to have certain properties like energy gaps for some given sizes of the quantum dots. In such situations, researchers prefer to carry out band gap engineering by changing the doping or alloying. In such situations, simulations are very useful to narrow down the time, money and efforts to identify the requisite materials. We have chosen CdSSe as our test materials to demonstrate the importance of this study.

Results

In the present work we have studied ten different sized (from 2.2 nm to 4.6 nm) spherical quantum dots of CdS_xSe_{1-x} with six doping values for the parameter x (x = 0.0, 0.15, 0.36, 0.63, 0.79, 1.00) as shown in the graph. Fitting parameter and bowing parameter b (highlighted with red) are shown in table. It is observed that bowing parameter b is slightly higher than bulk CdS_xSe_{1-x} alloy. These values will enable experimentalists to design specific sized quantum dot of CdS_xSe_{1-x} with desired energy gap for a particular application with a specific value of x



Size (diameter) 'd' (*nm*)	b	b'	b"	b+b'+b"	CdSe gap (*eV*)	CdS gap (*eV*)
2.20	0.32	0.16	2.98	3.46	2.98	3.47
2.40	0.33	0.14	2.80	3.27	2.80	3.29
2.60	0.34	0.14	2.71	3.19	2.71	3.21
2.80	0.32	0.17	2.61	3.10	2.61	3.11
3.00	0.31	0.18	2.51	3.00	2.51	3.02
3.20	0.34	0.16	2.44	2.94	2.43	2.95
3.40	0.32	0.19	2.39	2.90	2.38	2.90
4.20	0.33	0.20	2.17	2.70	2.17	2.71
4.40	0.32	0.18	2.13	2.63	2.13	2.65
4.60	0.32	0.21	2.11	2.64	2.10	2.66
bulk	**0.29**	**0.38**	**1.74**	**2.41**	**1.74**	**2.42**

Table : coefficient of fitting parameter of quadratic equation in x ; bx^2+b'x+b"

Impact

Our work gives insight to experimental people who are working with CdS_xSe_{1-x} alloy quantum dots to tune doping parameter and size to get desired HOMO-LUMO gap i.e. energy gap.

The knowledge of precise interaction mechanism of individual phonons with the inner nanostructure would lead to nanoscale motion control in nanomechanical and biotechnological applications.

How this research work is benefited using PARAM Yuva II

The calculations for size less than 3nm can be carried out on our departmental level HPC facilities, but size beyond that was not doable on our machine. Because of Param Yuva we can do calculation of quantum dots having size more than 3nm, which was the important size range for experimental people.

Experiences using PARAM Yuva II (system, support etc.)

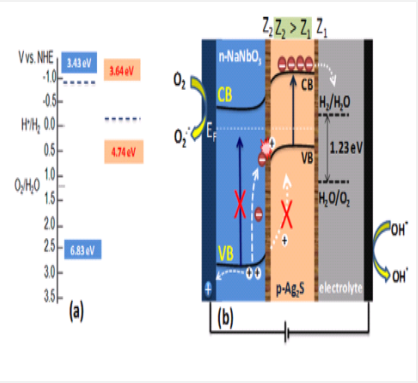
We have nice experience with PARAM Yuva II. We always get appreciable support from time to time from the user support team. Calculations in present work especially for larger quantum dots were not possible withput C-DACs valuable support.

Electronics and Thermal Properties of chalcogenide

CI: Dr. Abir De Sarkar abir@inst.ac.in

INSTITUTION: INST Mohali

RESEARCH DOMAIN: Material Science



Research Challenge

Research in clean energy generation is experiencing a global renaissance. The stringent environmental need for efficient and clean energy generation represents a strong pull to the scientific community. The largely improved experimental and theoretical tools to tailor materials, even on the nanometer scale, have now brought new imputes to the field, and enhanced international competition. In this proposed project we have theoretically investigate heterostructure compound for their potential in hydrogen generation and possible optimization of these materials by nanostructuring. Main challenges in this project are calculation of band structure of heterostructure and prediction of electron transfer path which is contributing in hydrogen evolving reaction.

Approach

We used density functional theory calculation to find the band structure of bulk materials. Then we perform work function calculation and band edge position for the heterostructure. From the band edge position of heterostructure we can define electron transfer path.

Results

The calculated density of states (DOS) and projected density of states (PDOS) of NaNbO3 and Ag2S are shown in Figure and explain a possible interband transition. This transition depends on the coupling between the valence-band and conduction-band states. A small DOS leads to small effective masses, which lead to a strong coupling between the valence- and conduction-band states of Ag2S. For NaNbO3, electrons are transferred from the occupied O2p states to unoccupied Nb 4d states under UV light; for Ag2S, electrons are transferred mostly from Ag3d states to the d conduction band. As excited-electron transfers from d to d states also have high backward transition rates, the photogenerated electrons can only migrate rarely to the surface and perform photocatalytic reactions. Owing to the high dielectric constant of NaNbO3 (∼20), an electronhole or polaron pair is weakly bound at the surface of the core material and dissociates quickly to form free charge carriers before recombination can occur.

Impact

The calculation is helpful to explain the experimental observation and it elucidate the

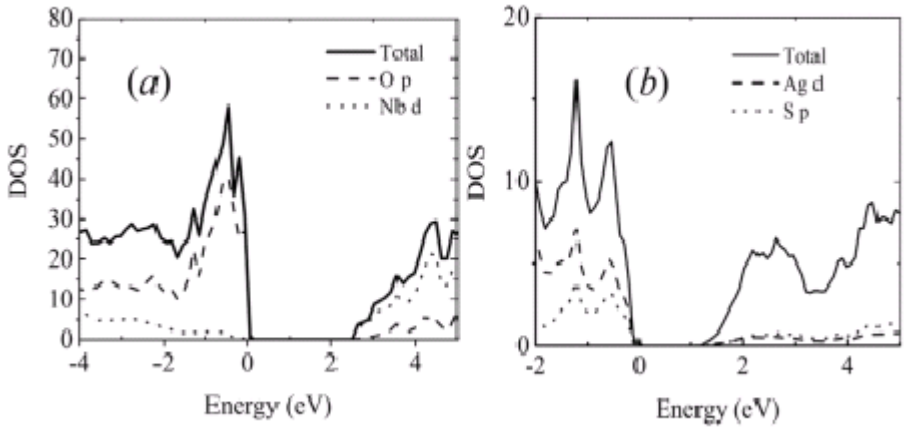


Figure: Total and projected density of states of (a) NaNbO3 and (b) Ag2S.

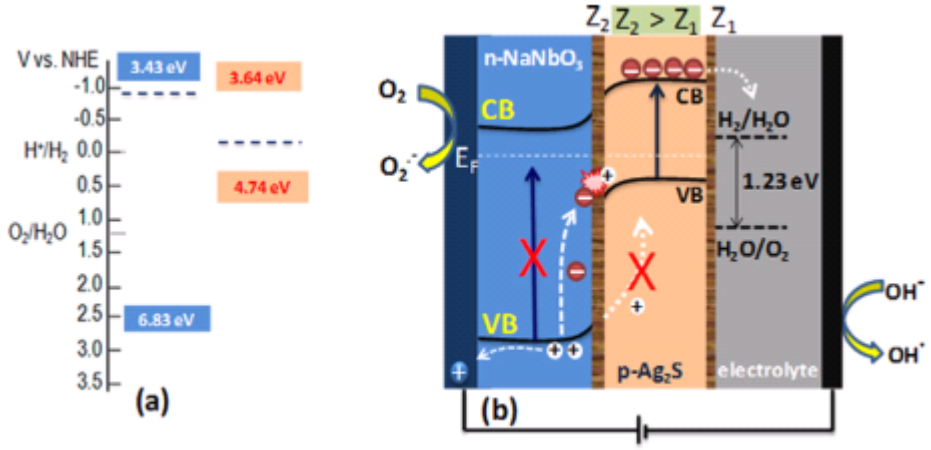


Figure: (a) Band-edge position and (b) the corresponding band diagram of the composite photoelectrode device.

mechanism behind the photocatalytic reaction under visible light.

How this research work is benefited using PARAM Yuva II

Support from PARAM Yuva II is very useful to perform the DFT calculation. With out PARAM Yuva II, it might not be possible to pursue the calculation

Experiences using PARAM Yuva II (system, support etc.)

We always get very supportive assistance from PARAM Yuva II team regarding installation of any software or setting and testing any new code. We are very thankful to PARAM Yuva II for the excellent support.

7

Ph.D Theses by PARAM Yuva II Users

Total number of Ph.D theses in Year 2016-17 : 09

1. **Molecular simulation study of triangle-well fluids confined inside slit pores**
   Student:Mr. Angan Sengupta, Department Of Chemical Engineering, Indian Institute Of Technology, Bombay
   Supervisor:Dr. Jhumpa Adhikari

2. **Rational Solvent Design for the Extraction of aPharmaceutical Intermediate, R-Phenylacetylcarbinol**
   Student:Ms. M. Harini, Department Of Chemical Engineering, Indian Institute Of Technology, Bombay
   Supervisor:Dr. Jhumpa Adhikari

3. **Edge effect on electronic band structure of graphene nanoribbons: A first principles study**
   Student:Ms. Deepika Goyal, IIT Ropar
   Supervisor:Dr. Rakesh Kumar

4. **Thesis Title : Not available**
   Student:Mr. Nityananda Sahu, IIT Kanpur
   Supervisor:Prof. Shridhar Gadre

5. **Thesis Title : Not available**
   Student:Mr. Anmol Kumar, IIT Kanpur
   Supervisor:Prof. Shridhar Gadre

6. **Molecular Dynamics Investigation of Fast Ion Transport in Oxide Frameworks**
   Student:Mr. Kartik Sau, Department of Physics, IIT Guwahati
   Supervisor:Dr. Padma Kumar Padmanabhan

7. **First Principles Investigations of Properties of Low Dimensional Systems and Their Role in Selective**
   Student:Ms. Indu Kaul, IISER Pune
   Supervisor:Dr. Prasenjit Ghosh

8. **On the likelihood of multiple errors due to neutron strikes:A circuit and layout perspective**
   Student:Ms. Nanditha Rao, Dept. of EE, IIT Bombay
   Supervisor:Prof. Madhav Desai

9. **Ab-initio calculations on electronic magnetic and lattice dynamical properties of Ni-Fe-Ga Heusler alloy**
   Student:Mr. Chabungbam Satyananda Singh, IASST
   Supervisor:Dr. Munima B Sahariah

8

Publications by PARAM Yuva II Users

Total number of publications by NPSF users in Year 2016-17 : 61

Publications by NPSF users

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

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

Nano Letters (13.779)

M. V. D. Prasad and B. Bhattacharya, Phonon Scattering Dynamics of Thermophoretic Motion in Carbon Nanotube Oscillators, Nano Letters, **16**, 2174-2180 (2016).

G. R. Yettapu, D. Talukdar, S. Sarkar, A. Swarnkar, A. Nag, P. Ghosh, and P. Mandal, THz conductivity within colloidal CsPbBr3 perovskite nanocrystals: remarkably high carrier mobilities and large diffusion lengths, Nano Letters, **16**, 4838 (2016).

Nanoscale(7.76)

Laxman Tatikondewar and Anjali Kshirsagar , Theoretical investigation of energy gap bowing in CdSxSe1-x alloy quantum dots. (*Submitted*)

ChemSusChem (7.116)

Kumar S., A P Singh, Chandan Bera, M Thirumal, B R Mehta, AK Ganguli, Visible-Light-Driven Photoelectrochemical and Photocatalytic Performance of NaNbO3/Ag2S Core Shell Heterostructures. ChemSusChem, **9**, 1850, (2016).

Scientific Reports (5.228)

Bedi R. K., Patel C., Mishra V., Xiao H., Yada R. Y. Bhaumik P., Understanding the structural basis of substrate recognition by Plasmodium falciparum plasmepsin V to aid in the design of potent inhibitors, Sci Rep., **6**, 31420, (2016).

Tushar Raskar, Sagar Khavnekar, Madhusoodan Hosur, Time-dependent X-ray diffraction studies on urea/hen egg white lysozyme complexes reveal structural changes that indicate onset of denaturation. Scientific Reports 6, Articlenumber:32277 (2016)

Deepika, Shailesh Kumar, Alok Shukla Rakesh Kumar, Origin of multiple band gap values in single width nanoribbons, Scientific Reports, **6**, Article number: 36168 (2016).

Journal of Molecular Biology(4.517)

Rajesh Kumar Kar, Hungyo Kharerin, Ranjith Padinhateeri and Paike Jayadeva Bhat, Multiple Conformations of Gal3 Protein Drive the Galactose-Induced Allosteric Activation of the GAL Genetic Switch of Saccharomyces cerevisiae, Journal of Molecular Biology, Volume 429, Issue 1, 6 January 2017, pp 158176 (2017)

Journal of Physical Cemistry C(4.509)

Rohit Babar and Mukul Kabir, Transition Metal and Vacancy Defect Complexes in Phosphorene: A Spintronic Perspective, J. Phys. Chem. C,**120(27)**, pp 1499115000 (2016).

Manasi S. Mahabal, Mrinalini D. Deshpande,Tanveer Hussain, and Rajeev Ahuja, Sensing Characteristics of Phosphorene monolayers towards PH3 and ASH3 gases upon the introduction of vacancy defects. J. Phys. Chem. C, **120**, 20428 (2016).

N. Kumar and P. Ghosh, Selectivity and Reactivity of Pd Rich PdGa Surfaces towards Selective Hydrogenation of Acetylene: Interplay of Surface Roughness and Ensemble Effect, J. Phys. Chem. C, **120**, 28654 (2016).

Physics Chemistry Chemistry Physics (4.449)

Seema Gautam, Abir De Sarkar, A systematic investigation of acetylene activation and hydracyanation of activated acetylene on Aun (n=3-10) clusters via density functional theory, Phys. Chem. Chem. Phys., **18**, 13830-13843 (2016).

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J. Cell. Biochem(3.446)

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J. Phys. Chem. B(3.187)

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Journal of Physical Chemistry A(2.693)

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Physical Review E(2.288)

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Journal of Biomolecule Structure and Dynamics (2.15)

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Materials Chemistry and Physics(2.101)

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Surface Science(1.931)

Manish K. Niranjan, *Theoretical investigation of surface states andenergetics of PtSi surfaces*, Surface Science, **649**, 2733 (2016).

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Chemical Physics(1.55)

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Journal of Molecular Modelling (1.438)

Venkataramanan N.S., Cooperativity of Intermolecular Hydrogen bonds in Microsolvated DMSO and DMF clusters: A DFT, AIM and NCI analysis, Journal of Molecular Modelling.

AIP Advances 6 (1.43)

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Weather (1.262)

Ancy Thomas, Sagar Kashid, Akshara Kaginalkar and Sahidul Islam, 2016: How accurate are the weather forecasts available to the public in India Weather,Vol. 71, No. 4, **84-88**, (2016).

J. Incl. Phenom. Macrocyclic Chem(1.253)

N.S. Venkataramanan, A. Suvitha, Structure, electronic, inclusion complex formation behavior and spectral properties of pillarplex, submitted to J. Incl. Phenom. Macrocyclic Chem.

Journal of Chemical Science (1.085)

S. R. Gadre, A. Kumar, Bonding and Reactivity Patterns from Electrostatic Landscapes of Molecules, J. Chem. Sci., **128**, 1519 (2016).

Mater. Res. Express (0.968)

Debashish Das, Shreemoyee Ganguly, Biplab Sanyal and Subhradip Ghosh, Effect of Fe doping in the structural, electronic and magnetic properties of CoCr 2 O 4: insights from ab initio calculations,Mater. Res. Express, **3**, 106106 (2016).

Advances in Condensed Matter Physics(0.9)

Priya Francis and S. V Ghaisas, Hydrogen terminated silicon nanoparticles with defects: A potential electrode for Li-ion battery, Advances in Condensed Matter Physics. (*Submitted*)

J. Phys.: Condens. Matter (0.8)

Debashish Das, Rajkumar Biswas and Subhradip Ghosh, Systematic analysis of structural and magnetic properties of spinel CoB 2 O 4 (B=Cr, Mn and Fe) compounds from their electronic, J. Phys.: Condens. Matter, **28** (2016) 446001.

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Soft Condensed Matter (0.621)

Indrajit Wadgaonkar, Apratim Chatterji, Network formation and gelation in Telechelic star polymers, Soft Condensed Matter , https://arxiv.org/abs/1609.08378

Conference Proceedings (2016-2017)

Nilesh Maltare and Chetan Chudasama, Applying parallel design patterns to embarassingly parallel problem. Colossal Data Analysis and Networking (CDAN), Symposium, DOI: 10.1109/CDAN.2016.7570888.

9

Visits to PARAM Yuva II

Total number of PARAM Yuva II visitors during Apr. 01,2016 - Mar. 15,2017 : 3607

Visits by dignitaries

- Shri. P. P. Chaudhary, Hon. Minister of State, Ministry of Law and Justice, Meity
- Shri. Anil Shirole, Hon. Member of Parliament, Pune
- Dr. Vijay Kumar Saraswat, Hon. Member of NITI Aayog
- Smt. Aruna Sundararajan, Hon. Secretary,Meity
- Dr. Aruna Sharma, Hon. former Secretary, DeitY
- Smt. Swetika Sachan, Assistant secretary, Meity
- Smt. Sarika Pradhan, Additional Secretary - MGNREGA/ RMDD, Govt. of Sikkim
- Shri. Umesh Prasad Sah, DIR-IT, Govt. of Jharkhand
- Shri. Sumnesh Joshi, Assitant Director General, UIDAI
- Shri. Anurag Tankha, Inspector General, NIA
- Dr. Dhananjay Ghanwat, Superintendent Of Police, Assam
- Smt. Renu Budhiraja, Sr. Director, Meity
- Shri. Sujit Banerjee, Scientist F, DST
- Dr. Subash Dhakal, OSD, MGNREGA/ RMDD, Govt. of Sikkim
- Shri. Ashis Chatterjee, HPC and Rack Scale Manager, Intel Corporation
- Shri. Arunava Roy Chowdhary, G.M., IREL
- Shri. U. C. Ray, Director at NIT MIZORAM
- Shri. Neeraj Kumar Gupta, Director, CEA
- Shri. V. V. Parlikar, Director, RDE, DRDO

- Lieutenant General, J S Cheema, DCOAS (IST), Indian Army
- Shri. Naveen Kumar, Deity

Table 9.1: Summary of Industrial Visits for students

Institution	No. of visitors	Visit Date
2016		
J K Institute of Applied Phy. and Tech., Allahabad Univ.	50	Apr. 12
Pimpri-Chinchwad College of Engineering	18	Apr. 13
INS Hamla, Malad, Mumbai	20	June 14
Deepstambh Foundation	-	July 22
Abhinav Education Society's CoET(Polytechnic), Satara	57	Aug. 25
D.Y.Patil Pratishthan Educational complex, Akurdi	80	-
AISSMS IoIT, Pune	67	Sept. 14
Shree Ramchandra College of Engineering, Pune	45	Sept. 19
Shri A.N. Patel Post Graduate Institute, Anand,Gujarat	53	Sept. 19
Don Bosco Institute of Technology, Mumbai	60	Sept. 22
Gharda Institute of Technology , Khed., Pune	40	Sept. 22
Trinity Polytechnic, Pune	60	Sept. 23
AISSMS IoIT, Pune	50	Sept. 26
Pratik Kharat	30	Sept. 26
Imperial College of Enigneering & Research, Wagholi, Pune	40	Sept. 27
MIT AOE, Pune	92	Sept. 27
Zeal Education Society's ZCOER, Narhe, Pune	80	Sept. 28
RMD Sinhgad School Of Engineering, Warje, Pune	90	Sept. 29
Rajarshi Shahu CoE, Pune	60	Sept. 30
VIIT Pune	60	Sept. 30
Govt. Polytechnic, Awsari	73	Oct. 03
PICT., Pune	62	Oct. 04
Marwadi Education Foundation	155	Oct. 04
Marathwada Mitra Mandal's Institute of Technology, Pune	64	Oct. 05
JSPM's Bhivrabai Sawant polytechnic, wagholi	70	Oct. 07
J T Mahajan College of Engineering, Faizpur	40	Oct. 07
St. Xavier's Engg. College, Ranchi, Jharkhand	70	Oct. 12
S.N.D.T. Arts and Commerce College for Women Pune	70	Oct. 13
Balasaheb Mhatre Polytechnic,Badlapur	30	Oct. 13
R.B.S Engineering Technical campus, Agra	70	Oct. 14
Terna Engg College	100	Oct. 14
Marathwada Mitra Mandal Polytechnic, Pune	120	Oct. 14
Dr. D. Y. Patil Institute for MCA, Akurdi, Pune	100	Oct. 17
M.P. COUNCIL OF SCIENCE AND TECHNOLOGY (MP-COST), Bhopal	130	Oct. 21
Ganpat University (GNU)	60	Dec. 14
Powar Public School	40	Dec. 15
VES College Mumbai	100	Dec. 19

Continued on next page

Table 9.1 – *Continued from previous page*

Institution	No. of visitors	Visit Date
VVS School	60	Dec. 21
B D Kale Mahavidyalaya	100	Dec. 27
PES, Modern college of Engineering	100	Dec. 28
2017		
Om Engineering College	40	Jan. 09
Abhinav College of Engineering, Satara	36	Jan. 13
Anjuman-I-Islam's Akbar Peerbhoy College of commerce and Economics, Mumbai	100	Jan. 17
MAREER's Arts, Com and Sc College, MIT, Kothrud	50	Jan. 23
M.L.Dahanukar College	140	Jan. 24-25
PG Diploma in IT, ACTS Student	60	Jan. 19
Gurukul Education Society Institute of Engineering & Tech.	40	Feb. 03
Faculty Development Program	20	Feb. 07
Dr. Y.S.Patil	15	Feb. 08
Latthe Polytechnic College	40	Feb. 09
Sinhgad Institute of Technology and Science, Narhe, Pune	60	Feb. 14
AISSMS IOIT Pune	65	Feb. 16
Armiet College	140	Feb. 17
Sree Narayana College, Kannur	12	Feb. 24
SN College, Mumbai	120	Mar. 02
MIT, Aurangabad	60	Mar. 06

Appendix A

Projects Enrolled during Year 2016-17

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

Table A.1: Projects using PARAM Yuva II compute time

Institution	Project	Chief Investigator	No. of users
Amity University	DFT based chemical, structural, optical and magnetic study of functionalized Graphene nanoribbons	Dr. Siddheshwar Chopra	1
	Computational Study of Arsenene based Nano-Devices	Dr. Manoj Kumar Sharma	1
Army Institute of Technology, Pune	Neural Network based Image Captioning	Dr. Nandkumar Bansode	5
Central University of Haryana	Ab initio Molecular Dynamics simulation of Ionic Liquid doped Polymer Electrolyte Membranes and Platinum Electrode Interface	Dr. Anurag Sunda	3
DRDO-BU Centre for Life Sciences,Coimbatore	Development of molecular simulation models for Biological therapeutic applications against target toxin agents	Dr. Venkataramana. M	4
D. Y. Patil University,Navi Mumbai	Investigation of cell division proteins in thermophiles	Dr. Debjani Dasgupta	3
GITAM School of Technology, Hyderabad Campus	Theoretical and observational study of cosmic molecules	Dr. Mahadev Naganathappa	1
GLA university, Mathura	Theoretical investigation of novel materials applications in the field of electronics and optoelectronic devices	Dr. Bramha Prasad Pandey	1
HPT Arts & RYK Sc. Coll., Nasik	Theoretical study of structural, electronic and magnetic properties of nanomaterials	Dr. Mrinalini Deshpande	2
	Electronic Properties of TM doped ZnO Sheet: Density Functional Study	Dr Mrinalini Deshpande	3

Continued on next page

Table A.1 – *Continued from previous page*

Institution	Project	Chief Investigator	No. of Users
IASST, Guwahati	New n-type organic semiconductors for optoelectronics: Synthesis, characterization and device fabrication	Dr. Sagar Sharma	1
IIA, Bangalore	Numerical simulations of Hydromagnetic turbulence from galaxies to Sun	Dr. Sharanya Sur	2
IIIT, Hyderabad	Simulation of Fault Motion Analysis, Simulation of Collapse behavior of buildings subjected to Earthquakes	Dr. Ramancharala Pradeep Kumar	3
IISER Pune	Molecular modelling and dynamics of polymers, gas hydrates and ionic liquids: An alternative energy initiative	Prof. Arun Venkatnathan	8
	Materials modelling at different length and time scales	Dr. Mukul Kabir	5
	Study of CdS and CdTeS quantum dots decorated on TiO_2 nanowires	Dr. Prasenjit Ghosh	7
	Selective hydrogenation of acetylene on Pd/Ga intermetallic compounds	Dr. Prasenjit Ghosh	3
	Catalyst design for molecular-H splitting	Dr. Mukul Kabir	3
	Vacancy diffusion in graphene	Dr. Mukul Kabir	2
	Microscopic mechanism for methane hydrate formation	Dr. Mukul Kabir	3
	O2 molecule splitting and diffusion on LaMnO3 surface	Dr. Mukul Kabir	3
IIT Guwahati	Atomistic simulation of fast ion transport in solids	Dr. Padma Kumar Padmanabhan	3
	Computational studies of allosteric mechanism of SAMHD1	Dr. Swati Bhattacharya	2
IIT Hyderabad	Structure and dynamics of RMA duplexes comprising of trinucleotide repeat expansion	Dr. Thenmalarchelvi Rathinavelan	1

Continued on next page

Table A.1 – *Continued from previous page*

Institution	Project	Chief Investigator	No. of Users
	Structure and dynamics of E.coli outer membrane lectin	Dr. Thenmalarchelvi Rathinavelan	2
	Calorimetric detection of UCHLI	Dr. Anindya Roy	2
	First Principles Investigation of Nano Materials	Dr. Amit Acharyya	3
Indian Institute of Technology, Indian School of Mines, Dhanbad	Three Dimensional modelling of Magnetotelluric Data over Dalma and Dhanjori Volcanics	Prof. Shalivahan	2
IIT Jodhpur	Chemical Dynamics Simulations of Complex Organic Reactions: Mechanistic Insights and Microsolvation Effects	Dr. Manikandan Paranjothy	2
	Numerical Simulation of large scale industrial bioreactor using GPU parallel algorithm	Dr. B. Ravindra	2
IIT Kharagpur	Computational Study of Enzyme Catalysis	Dr. Sabyashachi Mishra	3
	Analysis of Nano-composites using Molecular Dynamics	Dr.Mohammed Rabius Sunny	2
IIT Patna	Development of Smart Material using Molecular Dynamics Simulation	Dr. Sandip Khan	2
IKST (INDO KOREA Science and Technology Center)	Design of III-V semiconductor alloys for next generation electronics	Dr. Seung Cheol Lee	1
INAF	Flight Dynamics of Unpowered Glider	Air Marshal Shirish Deo	1
INST, Mohali	Atomic scale design of novel nanomaterials for clean energy and devices	Prof. Abir De Sarkar	5
	Ab initio molecular dynamics (AIMD) Simulations	Dr. Md. Ehesan Ali	1
	Electronics and Thermal Properties of chalcogenide	Dr. Chandan Bera	2

Continued on next page

Table A.1 – *Continued from previous page*

Institution	Project	Chief Investigator	No. of Users
	Quantum capacitance calculation of carbonaceous materials	Dr. Ramendra Sundar Dey	2
Kurukshetra University, Kurukshtra, Haryana	Simulations of rare earth free magnetic inorganic halide perovskites for photovoltaic applications, Academic	Dr. Manish Kumar Kashyap	3
NISER	Numerical Studies of correlated phases and transitions in frustrated magnets	Mr. V. Ravi Chandra	1
Pachhunga University College, Mizoram University	A first principles study of perovskite compounds, a probe for solar cell materials	Dr. Dibya Prakash Rai	1
SASTRA University	Inclusion Complexes of Cisplatin and its Analogues	Dr. A. Suvitha	1
Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab	Computational scrutiny of the mechanism of amyloid B-peptide aggregation	Dr. Bhupesh Goyal	4
SP Pune University	First-principles investigation of semiconductor nanostructures	Prof. Anjali Kshirsagar	2
	Water cluster and molecule interactions in electric field	Prof. Rajeev Pathak	2
	Probing noncovalent interactions using density functional theory	Prof. Shridhar P Gejji	3
	Probing noncovalent interactions in Ionic Liquids using density functional theory	Prof. Shridhar P Gejji	3
	Ab initio investigations on nano-biomaterials and ternary alloys	Dr. Vaishali Shah	5
	Effect of substitutional doping on electronic structure of II-VI semiconductor quantum dots	Prof. Anjali Kshirsagar	2
	Fractional Ordered Dynamical Systems	Prof. Varsha Gejji	2

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Table A.1 – *Continued from previous page*

Institution	Project	Chief Investigator	No. of Users
St. Xavier's College, Ahmedabad	Quantum transport in elemental doped boron nitride monolayer	Dr. Sanjeev Kumar Gupta	1
The Institute of Science, Mumbai	Materials for hydrogen storage	Prof. Ajay Chaudhari	2
THSTI, DDRC, Gurgaon	Functional characterization of finger loop with/without inhibitors in HCV RNA-Dependent RNA Polymeras	Dr. Shailendra Asthana	4
University of Hyderabad	Carbondionide capture and storage: Exchange with methane in clathrates	Dr. Manju Sharma	1
VNIT Nagpur	Quantam Information studies of condensed matter many-body sytems	Dr. M.S. Ramkarthik	2
	Understanding and Implementing Numerical Aspect of Fluid Flow and Heat Transfer in the Context of CFD for various applications	Dr. Trushar B. Gohil	5
	First priniciple study of some topological materials	Dr. Poorva Singh	2

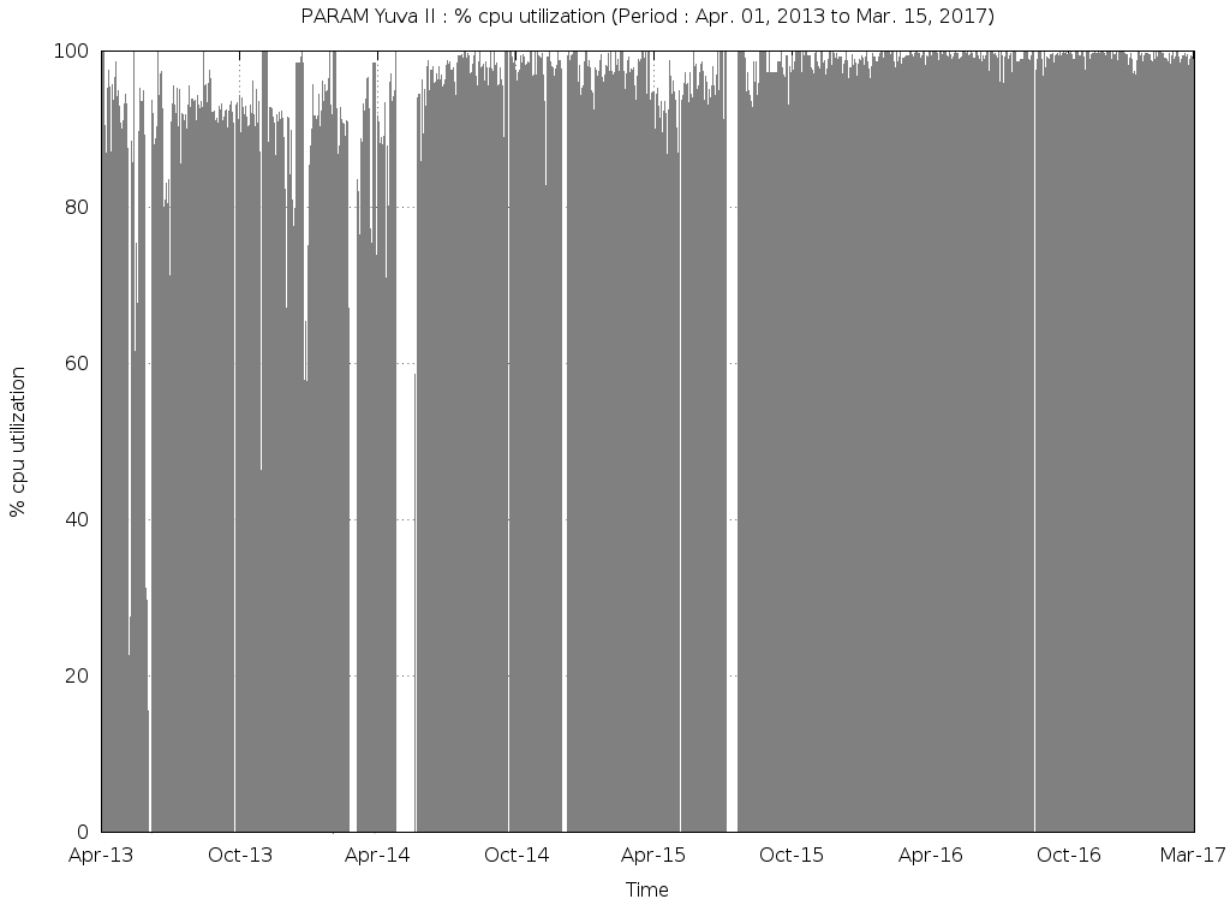
Appendix B

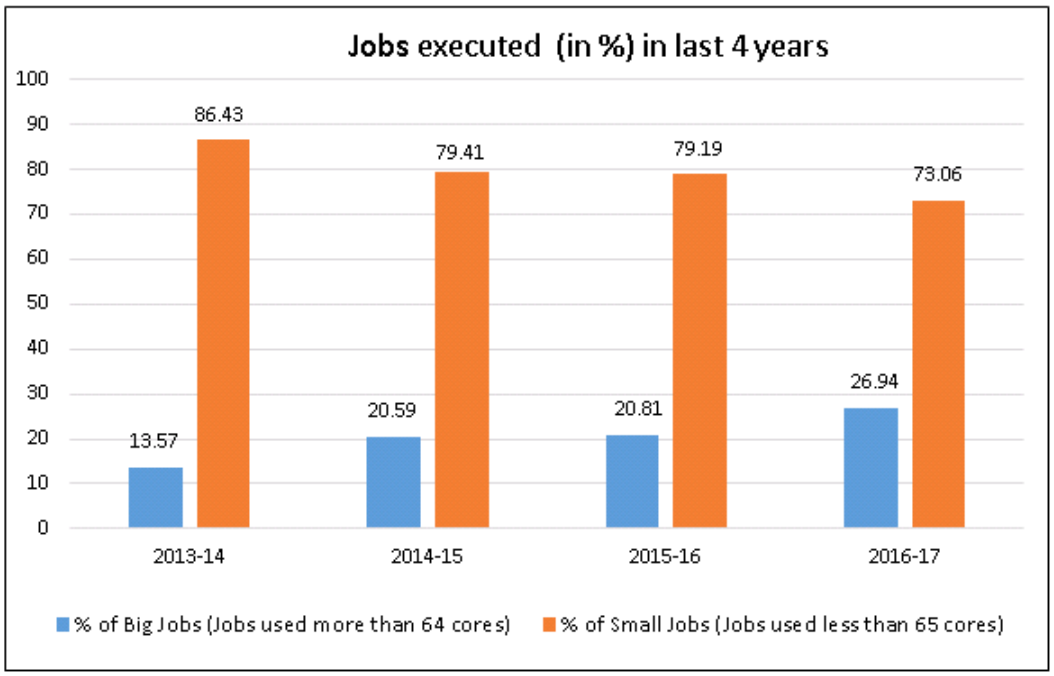
PARAM Yuva II Year 2013-17 Statistics

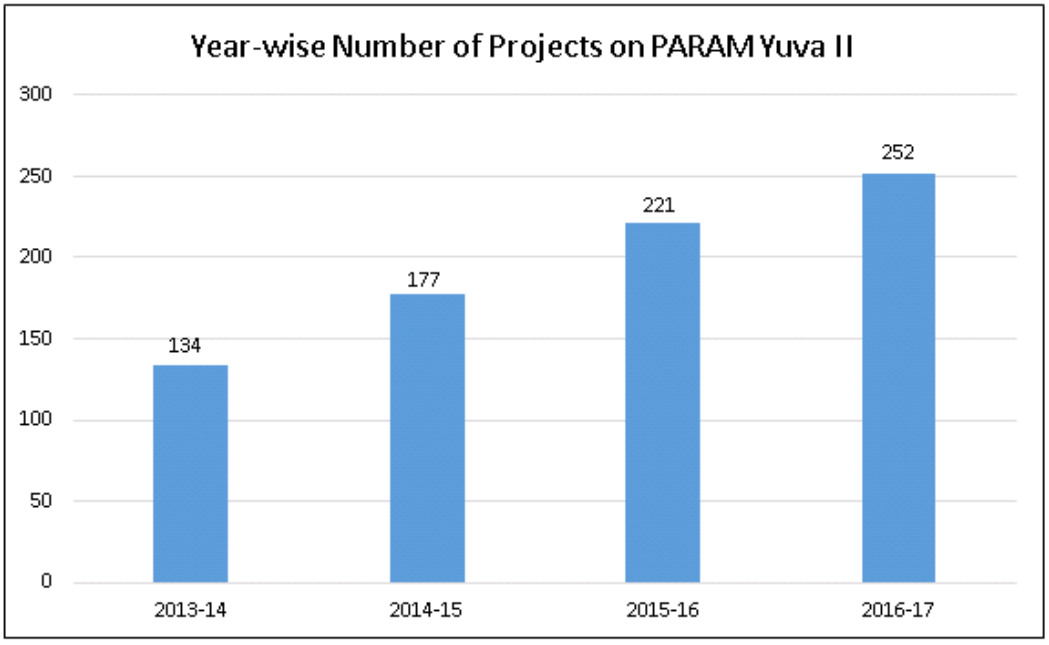
Below are some of the PARAM Yuva II statistics of last four years i.e Year 2013-17.

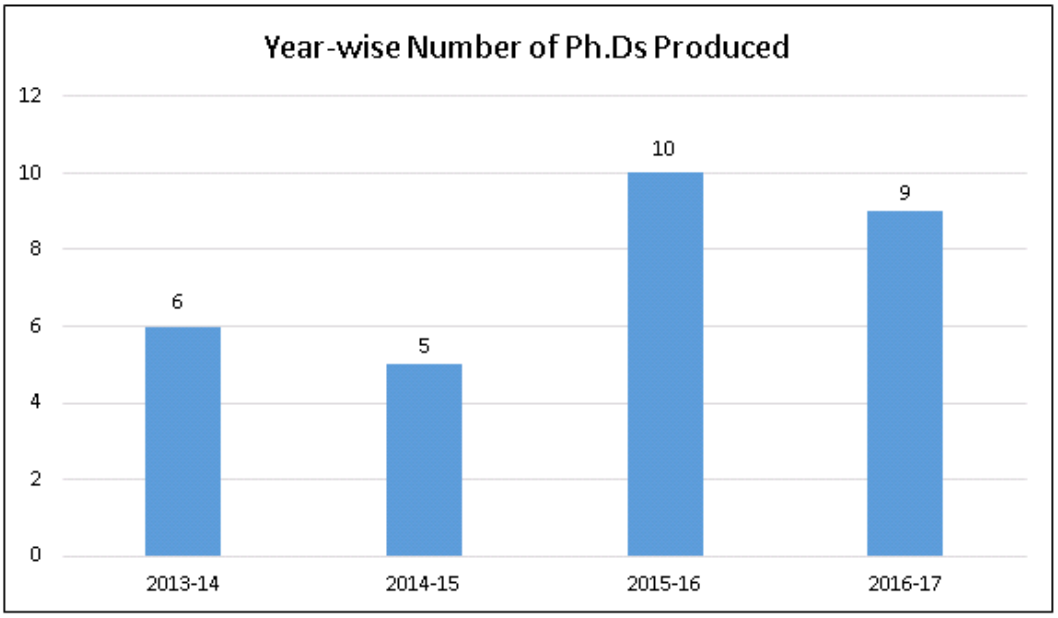
The statistics includes variation in cluster utilization, number of jobs executed, year-wise total number of projects, number of Ph.Ds & publications produced using PARAM Yuva II.

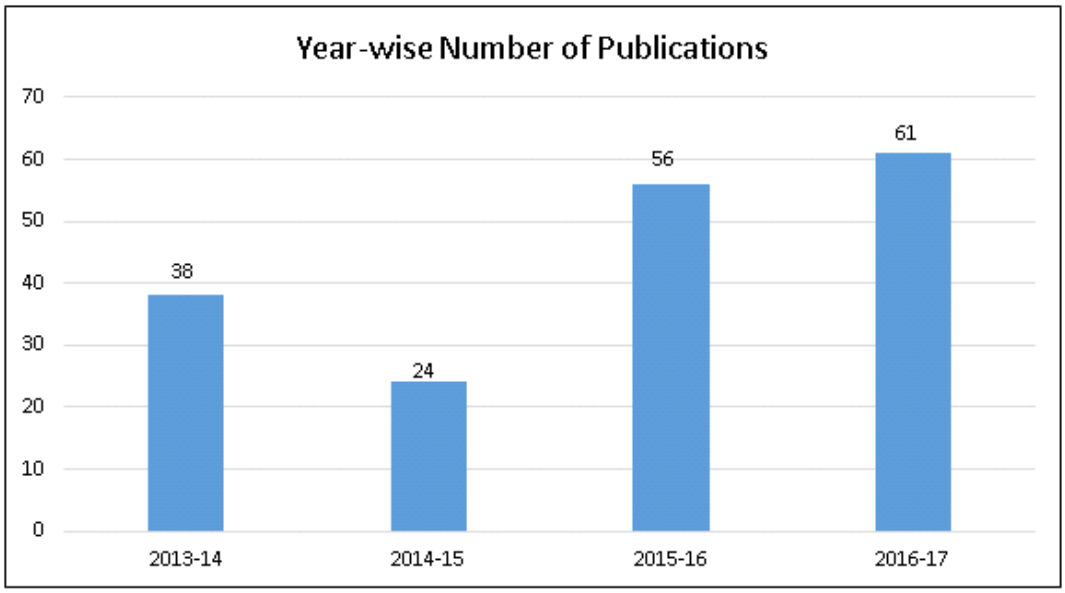
Below cluster utilization shows the year-wise increase in average cluster utilization.




Jobs executed (in %) in last 4 years
100
90
80
70
60
50
40
30
20
10
0
86.43
79.41
79.19
73.06
13.57
20.59
20.81
26.94
2013-14
2014-15
2015-16
2016-17
% of Big Jobs (Jobs used more than 64 cores)
% of Small Jobs (Jobs used less than 65 cores)


Year-wise Number of Projects on PARAM Yuva II
300
250
200
150
100
50
0
134
177
221
252
2013-14
2014-15
2015-16
2016-17


Year-wise Number of Ph.Ds Produced
12
10
8
6
4
2
0
6
5
10
9
2013-14
2014-15
2015-16
2016-17


Year-wise Number of Publications
70
60
50
40
30
20
10
0
38
24
56
61
2013-14
2014-15
2015-16
2016-17

Appendix C

User's Appreciations

Below are few of the PARAM Yuva II user's appreciation quotes

"As my students who are accessing PARAM Yuva gave me a positive feed back on the computing resources"

Dr. Gopalan Rajaraman ,
Prof. Amitabh Bhattacharya (Chief Investigator)
IIT Bombay

"I thank you from the bottom of my heart for all your help, guidance and patience. It is all your team's effort that researchers like me are able to do quality research."

Dr. siddheshwar chopra(Chief Investigator) ,
Amity University, Noida

"Our poster won the best poster award at Indian Biophysical Society conference which included work from PARAM YUVA II- dedicated slot."

Mr. Sagar Khavnekar ,
Dr. Avinash Kale (Chief Investigator)
CBS, Mumbai

"Another good news is that one more paper has accepted. I will furnish its details in a short span of time. All credit to you all. Thank you for supporting our research."

Dr. Siddheshwar Chopra (Chief Investigator),
Amity University, Noida

"I am highly obliged to C-DAC, Pune for providing the supercomputing facility. I have accessed the Gaussian-09 from C-DAC from August 2015-November, 30, 2015. Based upon that recently we have published results in PCCP successfully. Now I am doing my all research work using VASP in C-DAC's PARAM Yuva-II"

Dr. Seema Gautam,
Dr. Abir De Sarkar (Chief Investigator)
INST, Mohali

"I am thankful to CDAC people for their kind help. I also appreciate their efforts and support for helping scientific community."

Mr. Dimple Sharma,
Dr. Abir De Sarkar (Chief Investigator)
INST Mohali

"Congratulations to NPSF team. It is all your patience and support that has let us run all these jobs. Keep up the good work."

Dr. siddheshwar chopra (Chief Investigator),
Amity University, Noida

"Our experience of using PARAM-YUVA-II was very satisfactory during the period of MoU. We received good computational services and a very nice support from the CDAC staff. We greatly appreciate the services provided by CDAC."

Mr. Y. P. Rana,
SAC, ISRO

"It gives us enormous pleasure in communicating to you that a research Publication based on our recent research work has been accepted for publication in The Journal of Chemical Physics, published by the American Institute of Physics. The computations involved in the research work were carried out under the research scheme granted to us by C-DAC that employed the PARAM-YUVA high performance computing facility. The support by C-DAC has been crucial, without which the research would never have been materialized. We look forward to having your continued support."

Ms. Nalini Gurav,
Dr. Rajeev Pathak (Chief Investigator)
S P Pune University, Pune

"I feel happy to inform you all that I have got one more paper published recently. I thank all of you for helping us day in and day out. It is all possible due to your team's support."

Dr. Siddheshwar Chopra (Chief Investigator),
Amity University, Noida

"Over the past several years, the service I received by NPSF is immense and indispensable.My research, involving micron long atomic systems, would not have been possible without PARAM facility. I am extremely grateful for this and I have this feeling that, in future, I would like to contribute to PARAM in any possible way."

Mr. Prasad Matukumilli,
Dr. Baidurya Bhattacharya (Chief Investigator)
IIT Kharagpur

"We have recently published an article in Scientific Reports of Nature Publications. We have acknowledged your HPC facility as without it this work would not have been possible. I thank you again. Keep up the good work!"

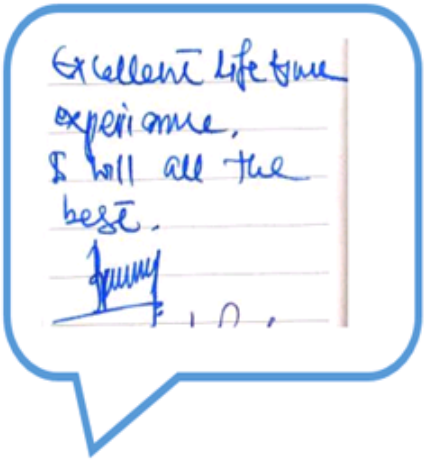
Dr. Chandan Patel,
Prof. Amitabh Bhattacharya (Chief Investigator)
IIT Bombay

"Thanks for your immediate assistance in this regard. Your help in extending my home area quota for this academic year also is greatly appreciated. I also thank the entire NPSF team for providing the required computational resources for scientific research and timely support during queries."

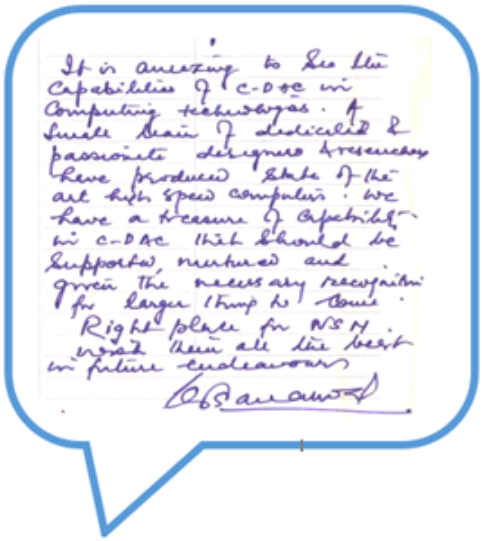
Mr. Yogesh Prasad M S,
Prof. Amitabh Bhattacharya (Chief Investigator)
IIT Bombay

Appendix D

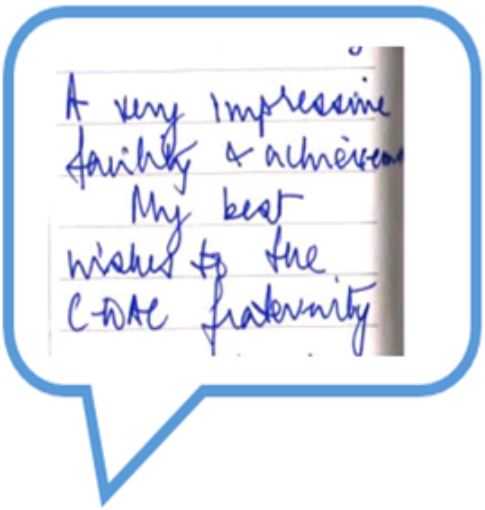
Visitor's Quotes



Shri. P. P. Chaudhary,
MOS, Law and Justice,
Ministry of Law & Justice & Ministry of Elect. & info. Tech.,
Govt. OF India

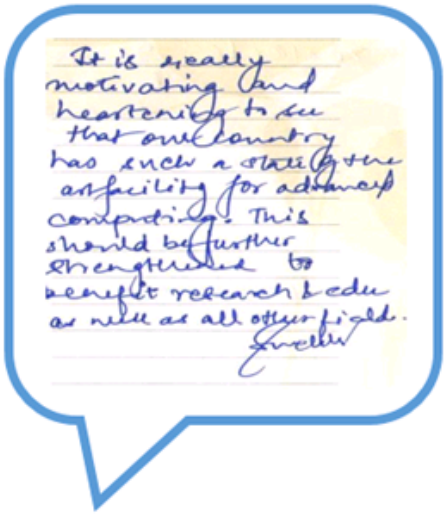


Dr. V. K. Saraswat,
Former Secretary Defense R&D,
Member, NITI Aayog , Govt. OF India



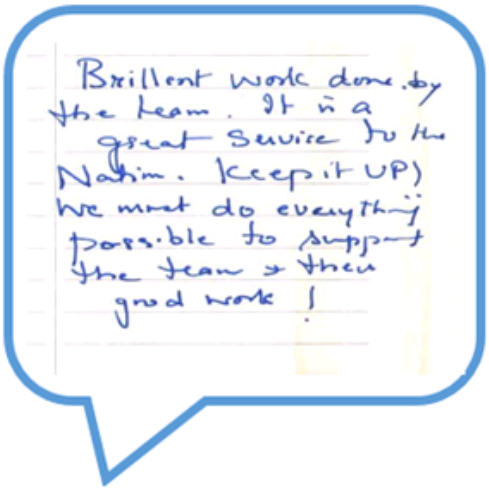
Smt. Aruna Sundararajan,
Secretary, DeitY, Govt. OF India

Dr. Aruna Sharma,
Ex-Secretary, DeitY, Govt. of India



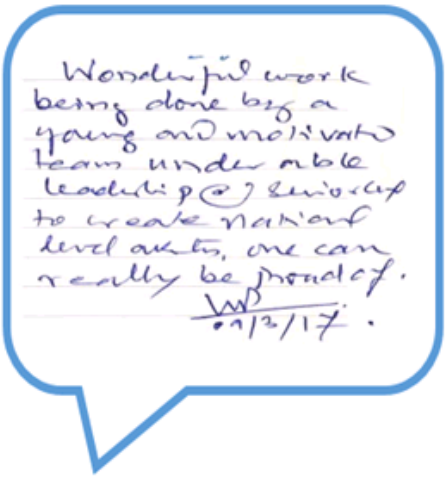
Smt. Swetika Sachan,

Assistant secretary, MeitY



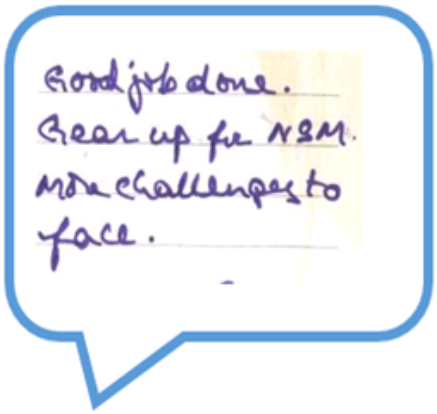
Smt. Renu Budhiraja,

Sr. Director, MeitY, Govt. OF India



Shri. V. V. Parlikar,

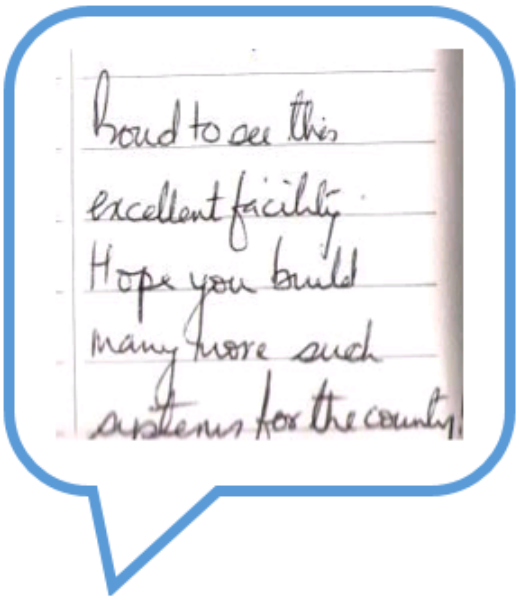
Director, R&DE (E), DRDO, Pune



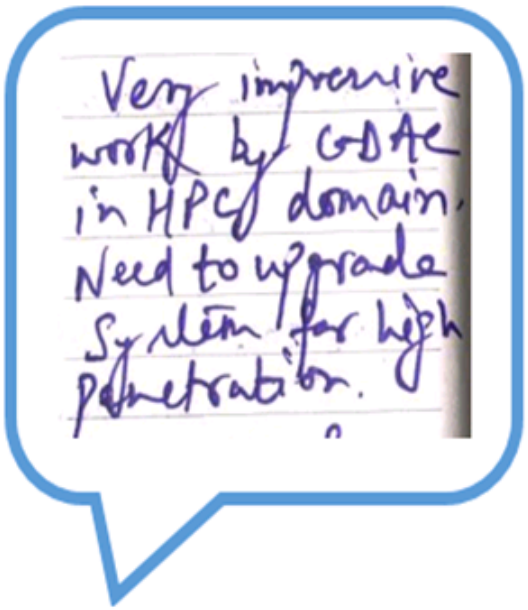
Shri. S. A. Kumar,

Scientist F, MeitY,

Govt. OF India



Dr. Sujit Banerjee,
Scientist F, DST,
Govt. OF India



Shri. Naveen Kumar,
MeitY, Govt. OF India

Appendix E

Picture Gallery

Visit to PARAM Yuva II by Shri . P. P. Chaudhary(6^{th} from left), Hon. Minister of State, Ministry of Law and Justice, Meity

Visit to PARAM Yuva II by Shri. Anil Shirole(3^{rd} from left), Hon. Member of Parliament, Pune

Visit to PARAM Yuva II by Dr. Vijay Kumar Saraswat, Hon. Member of NITI Aayog

Visit to PARAM Yuva II by Smt. Aruna Sundararajan, Hon. Secretary, Meity

Visit to PARAM Yuva II by Dr. Aruna Sharma (3^{rd} from left), Hon. former Secretary, DeitY

Ms. Shraddha Jani explaining about NPSF on National Science Day, C-DAC, Pune

Mr. Akash Dumbre explaining about NPSF on National Science Day, C-DAC, Pune

Mr. Pankaj Dorlikar explaining about NPSF on National Science Day, C-DAC, Pune

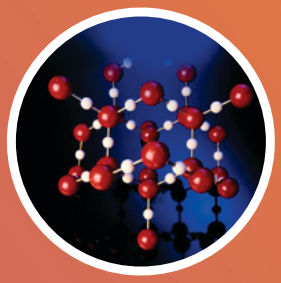
Ms. Nisha Agrawal explaining about NPSF on National Science Day, C-DAC, Pune

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

NPSF Operations Team, C-DAC, Pune

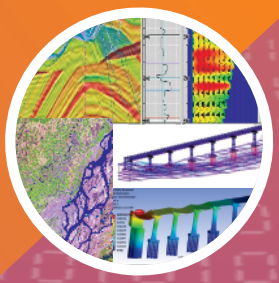
;

Space Applications



Basic Sciences

Data Sciences



Engineering Applications

Defence & Atomic Energy Applications

Earth Sciences

सी डैक
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पुणे विश्वविद्यालय परिसर, गणेशखिंड, पुणे - 411 007, भारत
Pune University Campus, Ganeshkhind, Pune 411 007, India.
फ़ोन / Tel: +91-20- 2570 4100, फैक्स / email: npsfhelp@cdac.in