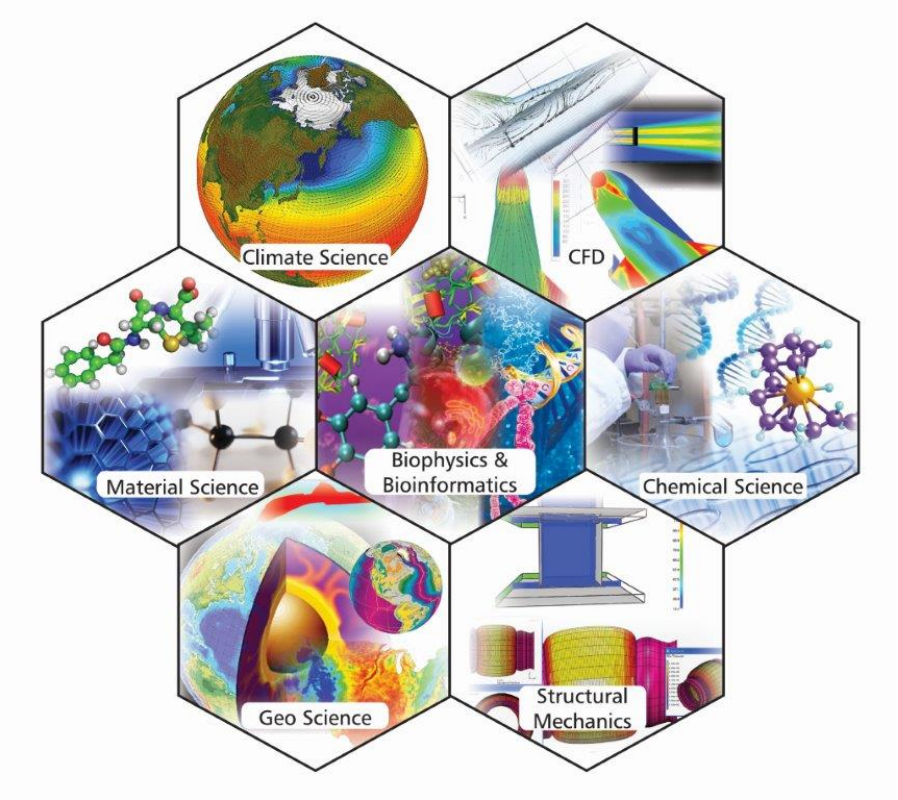
Annual Report
of
National PARAM Supercomputing Facility

NPSF
National PARAM Supercomputing Facility

2014-15



सी डैक
CDAC

Centre for Development of Advanced Computing, Pune

Message From Director General, C-DAC

Indian HPC community would be stepping into the Petascale computing era with the launch of the long awaited National Supercomputing Mission (NSM) soon. There would be emphasis on both capability as well as capacity computing leading to several computing systems of various scales across the country. It is very much essential to consolidate the efforts for the development of home grown applications on these emerging HPC platform to address the challenges before the nation. The areas of relevance could be disaster management, viz., flood/tsunami warning systems, earth quake engineering, high resolution weather prediction, development of new functional materials, drug design to name a few, which can lead to improvement in the quality of life of common man. C-DAC has a major role to play in terms of man power training and developing computing solutions in order to provide the required impetus to this national initiative.

At this juncture, it is worth mentioning that C-DAC's half Petaflop supercomputer PARAM Yuva II hosted at National PARAM Supercomputing Facility (NPSF) successfully completed two years of its commissioning on 8, February 2015. To commemorate this, NPSF had organized a workshop on Scientific Applications on PARAM Yuva II . The users from different domains presented their research work apart from sharing their experiences in using PARAM Yuva II. This workshop served as a forum bringing together the users and the NPSF team to take this partnership to the next level in future.

At present, over 650 users from 56 institutions are using PARAM Yuva II for their scientific work. 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. The compute power of the system at NPSF and their user base is expected to increase many fold in the years to come. They have a major role to play in supporting the end users to accomplish the quality of research expected using Petascale systems. This report summarizes the activities of the NPSF group during the year 2014-15 alongside showcasing the scientific activity by the users of this facility. I look forward to their wholehearted participation in C-DAC's initiative under the forthcoming NSM.

Prof. Rajat Moona
Director General, C-DAC

Message From Executive Director, C-DAC, Pune

The June of 2014 saw PARAM Yuva II crossing a major milestone of processing 1,00,000 jobs. PARAM Yuva II completed two years of computing resource support to the Indian scientific community in February this year. The NPSF had organized a workshop on Scientific Applications on PARAM Yuva II to mark this occasion. The workshop witnessed the participation of around 120 users from various domains. There were presentations by faculty members as well as students on the scientific work pursued using PARAM Yuva II. The enthusiastic participation reflected their deep sense of satisfaction in using our facility.

With the advent of National Supercomputing Mission, NPSF will continue to have world class facility to cater to the needs of data intensive computing. The expectations are high from the C-DAC HPC community under this national initiative. We shall continue our activity of user support, man power training and collaboration to help the proliferation of HPC in India, marching towards the Petascale computing era.

The NPSF team can take pride for their achievement in providing support to over 650 users from different institutions using this system for their research work. This user base is expected to grow by leaps and bounds in future years. I am confident that the dedicated staff at NPSF would continue their good work in the years to come. This report is a compendium of the activities of NPSF and the PARAM Yuva II users during the period 2014-15. I congratulate the NPSF team for their achievement in delivering the best of the computing facility to the Indian scientific community.

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

Message From HoD, NPSF, C-DAC, Pune

I am happy that PARAM Yuva II has completed two years of its commissioning in February 2015. It was a momentous occasion for us on achieving this milestone of supporting the PARAM Yuva II users for over two years as with other systems at NPSF in the earlier years. We decided to conduct a workshop to commemorate this, bring the user community together and learn about their experiences and expectations as NPSF users. We had a good response from the users for their participation in the workshop and present their research work carried out using our facility. The users strength of PARAM Yuva II is around 680 at present. This number would rise in future years for sure, given the fact that our team is working hard towards achieving high level of user satisfaction. Their efforts for improving the quality of service through efficient resource management, prompt resolution of support calls and user application support are laudable.

As we anticipate the launch of the National Supercomputing Mission, we need to prepare ourselves with new technologies, may it be HPC compute hardware, software, scheduling and resource management or power and cooling infrastructure that is required for running a larger facility. I understand that our team is keeping abreast of the technologies for future supercomputing centers which would help in planning our future activities. The NPSF along with other HPC groups of C-DAC would be expected to provide the leadership to various programmes under this initiative.

This report is a summary of our activities related to PARAM Yuva II facility management, user support in the year 2014-15. Some of the sections in this report showcase the scientific activities by users of PARAM Yuva II. I am confident that the NPSF team would deliver their best in offering a world class computing facility to the Indian scientific community for the years to come.

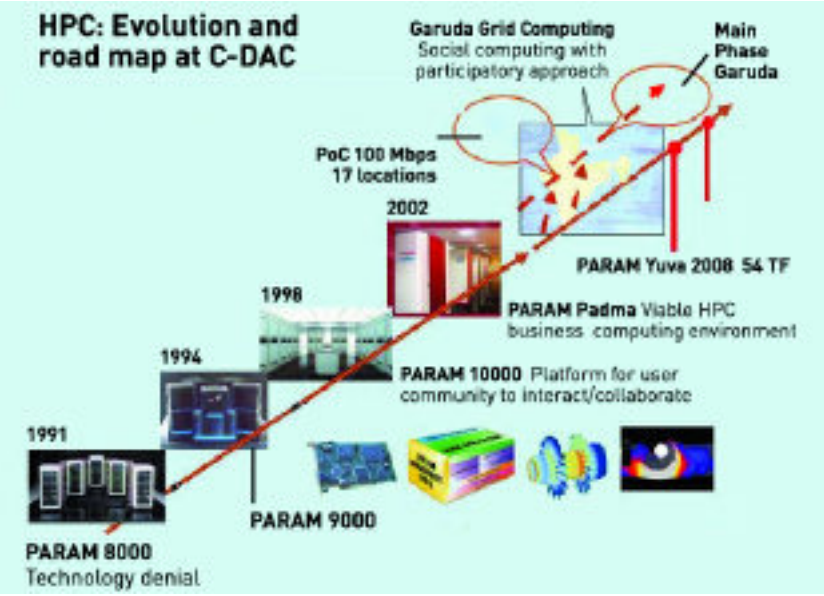
Mr. Sanjay Wandhekar
Associate Director & HoD, NPSF, C-DAC, Pune

Contents

1

Background

C-DAC is an R&D organization established with the primary objective of developing a supercomputer with a capability of one giga, or one billion, floating point operations a second (1 Gflops) in the early 1990s. Christened as PARAM 8000, it set the platform for a whole series of parallel computers, called the PARAM series of supercomputers, over the years. In 1998, PARAM 10000 with 100 GFlops peak performance set the path for future developments to come. With the commissioning of PARAM Padma, the Tera Flop (thousand billion Flops) barrier was broken in 2002 with a peak speed of 1 TFlop. The next one in this series was PARAM Yuva (henceforth referred as PARAM Yuva I), which was built and launched in 2008. It ranked 68^{th} in the TOP500 list released in November 2008 at the Supercomputing Conference in Austin, Texas, United States.



PARAM Yuva I relied on high-speed 10 gigabits per second (Gbps) system area network called PARAM Net-3, developed indigenously by C-DAC. This HPC cluster was built with nodes designed around state-of-the-art architecture known as x86 based on Quad Core processors. In all, PARAM Yuva I, in its complete configuration, had 4,608 cores of Intel Xeon 7350 processors called Tigerton with a clock speed of 2.93 gigahertz (GHz). The system had a sustained performance of 37.8 TFlops and a peak speed of 54 TFlops.

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.

C-DAC had set up a National PARAM Supercomputing Facility (NPSF) in 1998 at C-DAC, Pune to **facilitate the access to HPC resources** for *researchers around the country required to solve compute-intensive problems.* 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/Intitute/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.* Please refer to NPSF portal `https://npsf.cdac.in/` for details.

This report documents the activities of NPSF undertaken during 2014-15.

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Current Project by NPSF

The activities of the National PARAM Supercomputing Facility were supported by the grant-in-aid financial support from DeitY, Ministry of Communications and Information Technology, Government of India. The brief details of the ongoing project is listed below with their deliverables / milestones.

1. **Provisioning of hybrid technologies in National PARAM Supercomputing Facility and C-DAC's Terascale Supercomputing Facility - A step towards Next Generation HPC** (DIT/R&D/C-DAC/2(1)/2011, dt. 29/03/2012)

   [Duration: 01/04/2012 - 31/03/2015, Status: Ongoing]

   Focus:

   - Upgrade of PARAM Yuva I nodes with accelerators/Many Integrated Cores
   - Cluster health monitoring and user support
   - Porting scientific applications and libraries upon user request
   - Development of PARAM Yuva collaborative environment
   - Development of tools and utilities for cluster management and utilization
   - Development of tools and utilities for High performance shared storage

Acknowledgment: We gratefully acknowledge the funding of these projects by DeitY, Ministry of Communications and Information Technology, Government of India. Also, we express our sincere gratitude to the members of the PRSG committees who have guided and supported the activities of NPSF.

3

Activity Highlights

2014

April
Major revamping of cluster partitions and file system of PARAM Yuva II undertaken during three weeks long maintainence period starting from Apr. 24.

May
Major revamping activity of cluster partitions and file system of PARAM Yuva II continued till May 16.

June
The jobs processed by PARAM Yuva II crossed 1,00,000 mark on Jun. 18 (since its commissioning on Feb. 8).

Mr. Sanjay Wandhekar partipated in the **International Supercomputing Conference** (*ISC '14*) between 22-26, held at Leipzig, Germany.

July
Prof. Jasjeet S. Bagha, IISER, Mohali visited NPSF on Jul. 2 and interacted with some members of NPSF on the details of PARAM Yuva II cluster. He also explored the possibility of collaborations between C-DAC and IISER, Mohali on HPC activities.

Dr. Manish Agarwal and Prof. Subodh Kumar from IIT, Delhi visited C-DAC between Jul. 14-15 and interacted with some mebers of NPSF team on operations and management of PARAM Yuva II.

Mr. Sanjay Wandhekar and Mr. Y. S. Swarup visited Intel Labs, Bangalore on Jul. 17 as part of technology update programme.

August
Dr. Sandeep K. Joshi delivered webinar titled "PARAM Yuva II Green 500 Level 3 benchmarking exercise" on invitation from the Chair of the *Energy Efficient HPC Working Group*, Ms. Natalie Bates, Lawrence Berkeley National Laboratory, USA on Aug. 5.

Mr. Rishi Pathak, Dr. Sandeep K. Joshi, and Dr. V. Venkatesh Shenoi delivered talks in the **HPC workshop** for *Ghana participants*, organized by High Performance Computing

Solutions group of C-DAC, Pune on Aug. 11-12.

September
Maintenence activity of PARAM Yuva II undertaken between Sep. 17-22.

October
Dedicated Slot Booking announced on Oct. 28 for the period from Nov. 15, 11.00 Hrs to Dec. 30, 11.00 Hrs.

Novemeber
Mr. Srinivasa Prasanna from IIA, Bangalore visited C-DAC between Nov. 12-24 for carrying out the performance tuning analysis of UTChem, a relativistic quantum chemistry code on PARAM Yuva II, along with Ms. Nisha Agarwal and Mr. Rishi Pathak.

Mr. Sanjay Wandhekar partipated in the **International Conference on High performance Computing, Network, Storage, and Analysis** (*SC '14*) between 16-21, held at New Orleans, LA, USA.

December
Dedicated Slot Booking for regular slots announced on Dec. 10 for the period from Dec. 30, 11.00 Hrs to Mar. 15, 11.00 Hrs.

Mr. Maneesh Kumar represented NPSF (as part of C-DAC stall) showcasing the activities of NPSF related to PARAM Yuva II in the exhibition during the 11^{th} IEEE India conference **INDICON 2014** conference (between Dec. 11-13) held at Pune.

Dignitaries at NPSF section of the C-DAC stall.

Paper titled "CFD simulation studies of high performance computing facilities" coauthored by Dr. Sandeep K. Joshi along with the colleagues from Computer Aided Engineering Group was presented in the 5^{th} **International and** 41^{st} **National Conference on Fluid Mechanics and Fluid Power** held at IIT, Kanpur between Dec. 12-14.

Dedicated Slot Booking for slots (in chunks of 16 hrs 55 minutes duration from 17.00 Hrs) announced on Dec. 24 for the period from Jan. 5 to Mar. 16.

2015

January
Workshop on **Scientific Applications on PARAM Yuva II** was organized by NPSF on Jan. 8-9, at IITM, Pune. There were invited talks and presentations by users of PARAM Yuva II (including C-DAC members) highlighting the scientific work carried out by them.

February
NPSF team participated in National Science Day celeberations at C-DAC on Feb. 28 showcasing the activities related to PARAM Yuva II to the students from Colleges and Schools in Pune.

School students at NPSF stall.

March
Computing resources support for HPC competition as part of Techkriti '15 organized by IIT, Kanpur between Mar. 19-22 2015.

4

PARAM Yuva II Highlights

Facts & Figures

- Date of commissioning: February 8, 2013
- Theoretical peak performance: 529.4 Tera Flops
- Sustained performance of 386.7 Tera Flops
- Computing power boosted by Intel Xeon Phi coprocessor technology
- Energy efficiency: 1,760.20 MFlops per Watt

Highlights

- **Completion of processing 1,42,420 jobs** (as of March 15, 2015)
  The jobs processed by PARAM Yuva II crossed 1,00,000 mark on June 18, 2014.
- **Top500 Ranking** `http://www.top500.org`
  Rank 131 as per November, 2014 Top500 list [Highest Rank: 69 in June, 2013]
- **Green500 Ranking** `http://www.green500.org`
  Rank 66 as per November, 2014 Green500 list [Highest Rank: 44 in Novemeber, 2013]
- **Completion of two years of commissioning**
  PARAM Yuva II *completed two years of commissioning* on February 8, 2015. The NPSF group had organized a workshop on **Scientific Applications on PARAM Yuva II** on January 8-9, at IITM, Pune to commemorate this.
- **User base**
  Around *689 users acoss 56 institutions avail computing time* on PARAM Yuva II for their scientific research.
- **External projects**
  Computing resources support for around 116 Projects[1] with Chief Investigators from Universities, IITs, and R&D institutions.
- **Ph.D students**
  Around *110 Ph.D students* are availing computing time on PARAM Yuva II for their thesis work. As of now, *10 students have completed their Ph.D thesis work* (including PARAM Yuva I).

[1] Please refer Appendix A for the complete list of projects.

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Computing Resources

A view of the computing facility.

HPC Cluster: There are **Four** subclusters constituting PARAM Yuva II,

- Subcluster 1:
  - **220 node cluster** of Intel server system R2000GZ
  - Dual socket Intel Xeon E5 2670 (Sandy Bridge) Processor
  - Eight CPU cores, 2.6 GHz
  - Two Intel Xeon Phi 5110P per node
  - Infiniband FDR interconnect
  - Partitions: FDRp, BIGJOBp, DEDp, DED2p

- Subcluster 2:
  - **Over 100+ node cluster** of HP Proliant DL580 G5
  - Quad socket Intel Xeon X7350 Processor
  - Four CPU cores, 2.93 GHz
  - System interconnects: PARAMNet3, Infiniband DDR
  - Partition: DDRp
- Subcluster 3:
  - **Four node cluster** of Supermicro SuperServer 1027GR-TRF
  - Dual socket Intel Xeon E5 2650 (Sandy Bridge) Processor
  - Eight CPU cores, 2.6 GHz
  - Two NVIDIA GPU Tesla M2090 per node
  - Infiniband FDR interconnect
  - Partition: GPUp
- Subcluster 4:
  - Supermicro 4U AMD SR5690 **SMP server** (64 cores)
  - Quad socket AMD Opteron 6276 Processor
  - Sixteen CPU cores, 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: Cent OS v6.2, Kernel v2.6.32-220
- Intel Cluster Studio XE 2013
- PGI Cluster Development Kit

Applications:

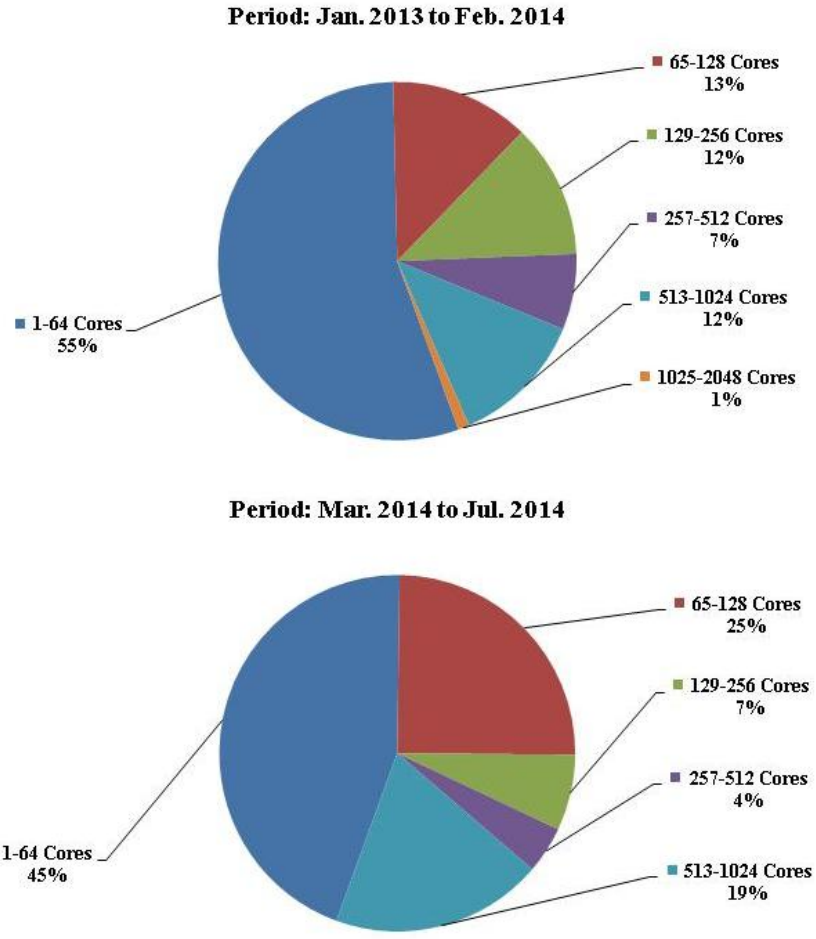
- Libraries and software for file formats, data bases and math
- Over 27 scientific applications for material science/quantum chemistry, molecular modelling, fluid dynamics, climate modelling and circuit simulations

There has been no addition to the computing resources (hardware) on PARAM YuvaII ever since the commissioning in Feb. 2013. However, *the cluster partitions have been created in order to improve the quality of service.*

Partitions and Queues:

The resources on PARAM YuvaII are grouped into homogenous groups known as partitions. To begin with, the partitions were: (1) DDRp, (2) FDRp, (3) GPUp, and (4) DEDp. The job submission queues were: (1) batch (2) GPUq, and (3) DEDq. Each of these partitions are mapped to different *job queues* with their respective *wall time* limit. The prominent changes based on the usage and scheduling policy are listed below:

- With the creation of TESTp partition, the users get resources without having to wait longer to run the test jobs before the actual job runs due to wall time restriction of 2 Hrs for TESTq queue.
- The queue wait time for the jobs with resource request of more than 64 cores has reduced considerably with the introduction of BIGJOBp partition, still ensuring better utilization of various partitions mapped to the batch (default) queue.



The data for the period from March to July, 2014 is compared with the ones till March 2014. The change in scheduling policy implemented in March 2014 had led to *an increase in the share of CPU time of the jobs requesting more than 64 cores* on PARAM YuvaII.

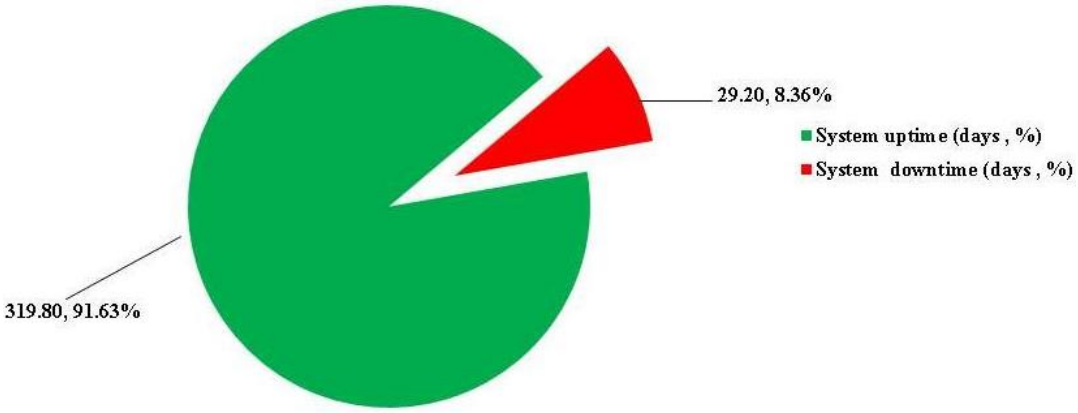
- The reservation of resources in the DEDp partition under Dedicated Slot Booking Facility (DSBF) through NPSF web portal has been made available for the users.
- The resources in the DED2p partition are primarily for running the production jobs on daily basis for a fixed duration as per the commitment to different users. The resources in this partition *during their idle time* have been made available to other users for reservation through DSBF.

Table 5.1: Summary of queues and partitions on PARAM Yuva II

Queue	Wall Time Limit	Associated Partition(s)	Accelerator(s) in the nodes in the partition
batch	7 Days	DDRp FDRp, BIGJOBp	 Xeon Phi
GPUq*	7 Days	GPUp	GPU
TESTq	2 Hours	TESTp	Xeon Phi
DEDq†	15 Days	DEDp	Xeon Phi
DED2q†	16 Hours 55 Minutes‡	DED2p§	Xeon Phi

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

PARAM Yuva II availability: (Period: Apr. 01, 2014 - Mar. 15, 2015) [349 Days]



- Uptime: ≈ 320 Days
- Maintenance Period: ≈ 29 Days
  - Apr. 24, 2014, 01:38 PM - May 16, 2014, 12:56 PM [21 Days, 22 Hrs]
  - Sep. 15, 2014, 11.00 AM - Sep. 22, 2014, 05:45 PM [7 Days, 6 Hrs]
- System uptime: ≈ 92%

*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.

6

Projects, Users, Usage & User Support Statistics

Projects & Users (as of 15^{th} March 2015)

- Number of projects : 177
- Number of users: 689 (across 56 Institutions)
- Number of PhD students: 115

Users across Institutions

Table 6.1: Users across Institutions

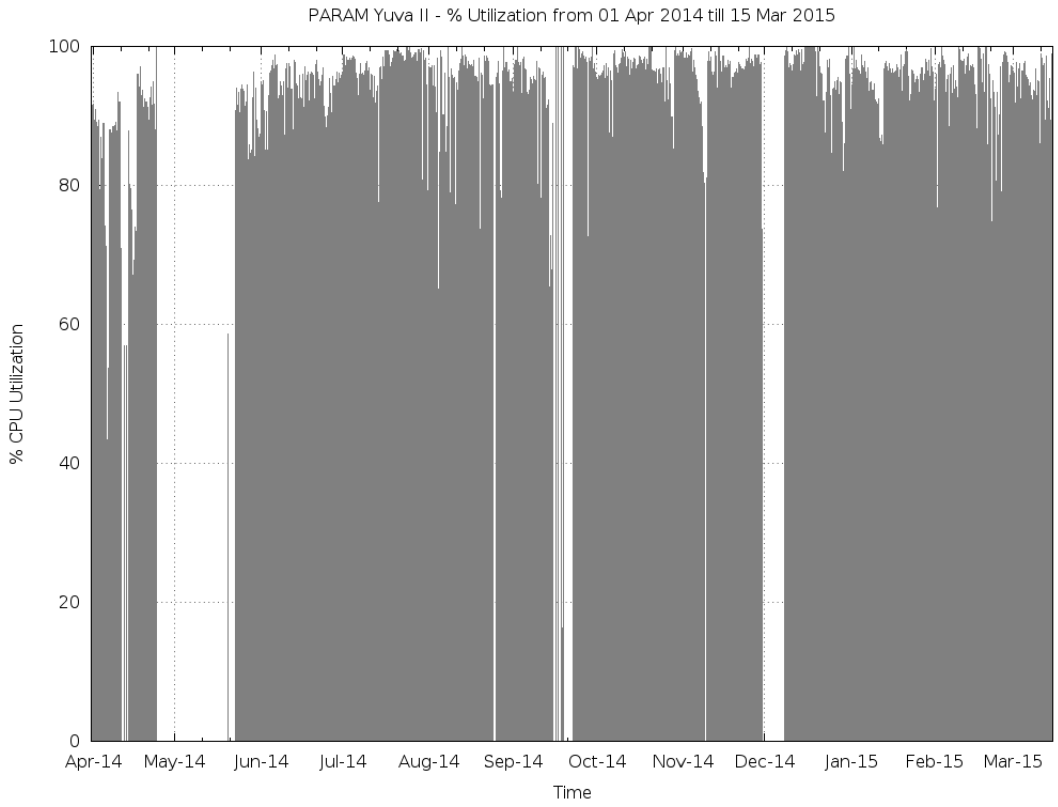
Institution	No. of Users
Ahmednagar College	1
Amity University	1
Anna University	2
BARC, Mumbai	1
CBS, Mumbai	2
CIFRI, Kolkatha	2
CMR College of Eng. & Tech	2
Carnegie Mellon University	1
C-DAC	115
CECRI, Karaikudi	1
Central Univ. of Bihar	1
Central Univ. of Gujarat	3
Delhi University	2
GARUDA	158
Govt. College, Tonk	1
Gunanak Dev University	1
Himachal Pradesh Univesity	3
HPT Arts and RYK Science College, Nasik	2
IASST, Guwahati	3
IIA, Bangalore	10
IIIT, Delhi	4

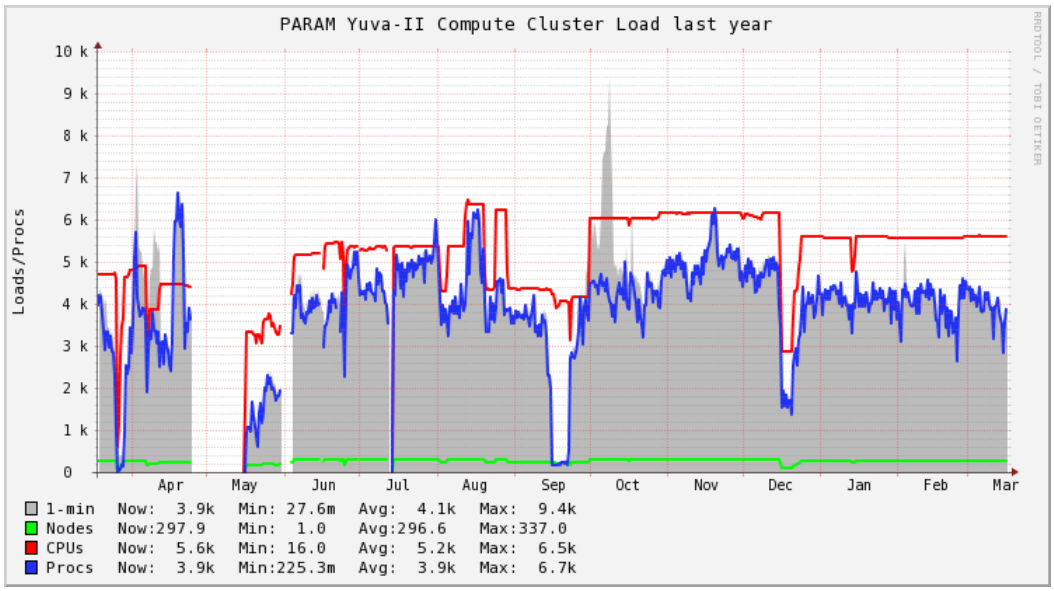
Continued on next page

Table 6.1 – *Continued from previous page*

Institution	No. of Users
IISc, Bangalore	7
IISER, Pune	40
IISER, Mohali	1
IISER, Thiruvananthapuram	3
IIT Bhubaneswar	2
IIT Bombay	151
IIT Delhi	5
IIT Guwahati	18
IIT Gandhinagar	8
IIT Hyderabad	7
IIT Jodhpur	3
IIT Kanpur	18
IIT Kharagpur	7
IIT Patna	4
IIT Ropar	8
INST, Mohali	5
ISRO	5
IUCAA, Pune	5
JMI, Delhi	1
Jiwaji University	3
JNCASR, Bangalore	8
JNU	2
MIT, Pune	1
Manipal University	2
NABI, Mohali	1
NCL, Pune	6
NCRA, Pune	6
NIC	2
NIT Calicut	1
NIT Rourkela	1
PRL, Ahmedabad	3
RRI, Bangalore	3
RTM Nagpur University	2
SP Pune University	23
SRM University	3
St. Xavier's College, Ahmedabad	1
Vijay Kumar Foundation, Gurgaon	6
VNIT Nagpur	1
Total	689

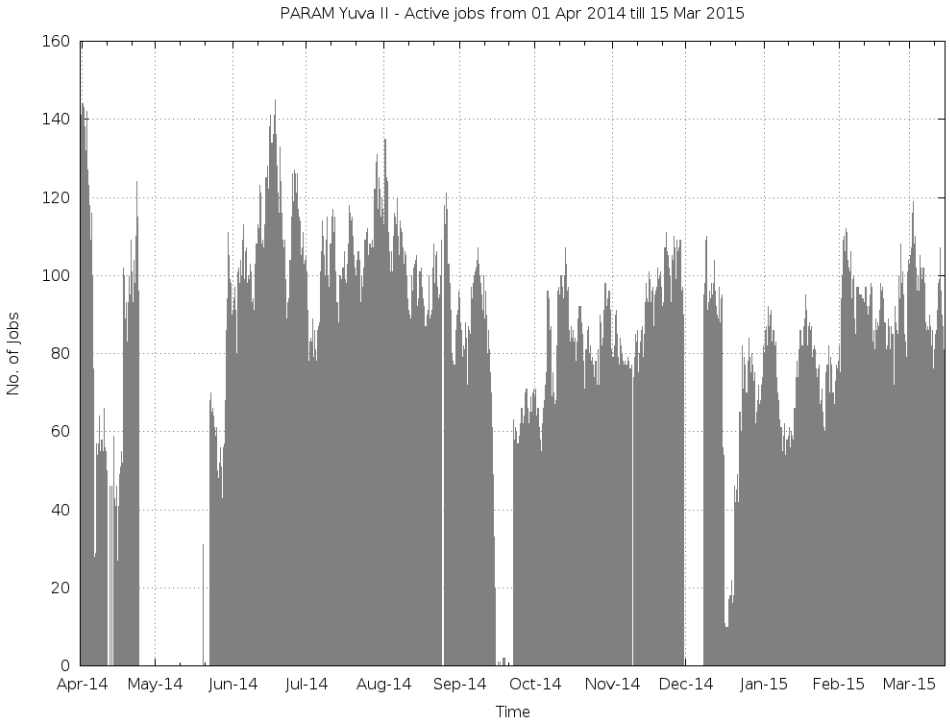
PARAM Yuva II System utilization:



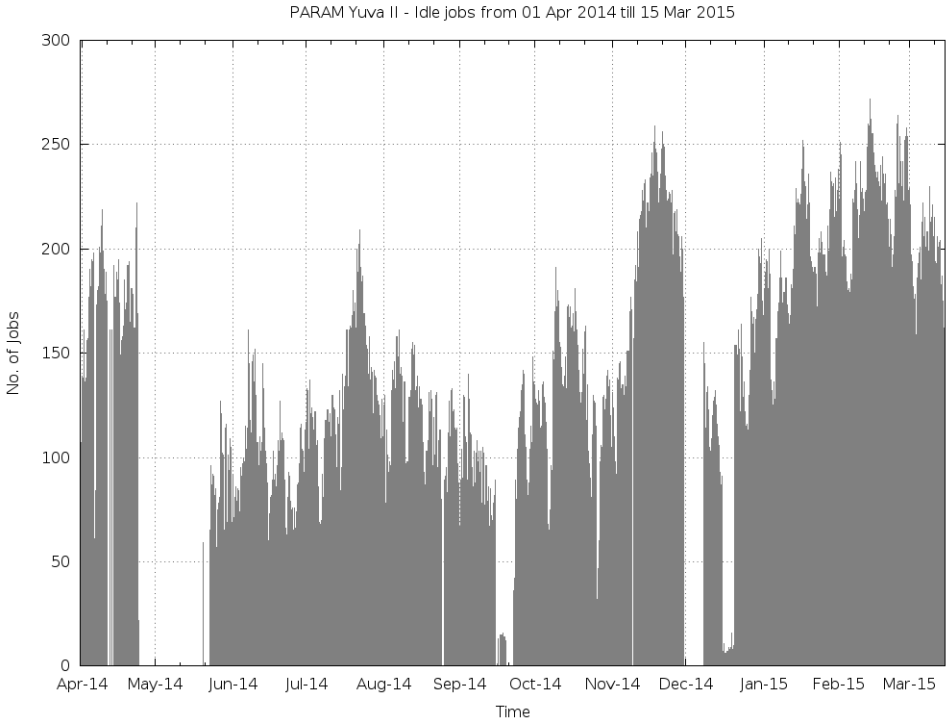


The maintenence activity of PARAM Yuva II accounts for the gaps in the months of April-May (21 days from Apr. 24) and September (7 days from Sept. 15) in the utilization graph (top). There was a partial shutdown of PARAM Yuva II (some of the nodes) for about 10 days during the month of December due to issues related to power and cooling infrastructure. This had hampered the data collection system also. This is reflected in the gap (missing data) in the utilization graph (top) in the beginning of December 2014. However, the partial shutdown during this period is reflected in the depletion of CPU cores as reflected from the complementary data from Ganglia (bottom).

Job Queues: Running Jobs (Active Jobs)



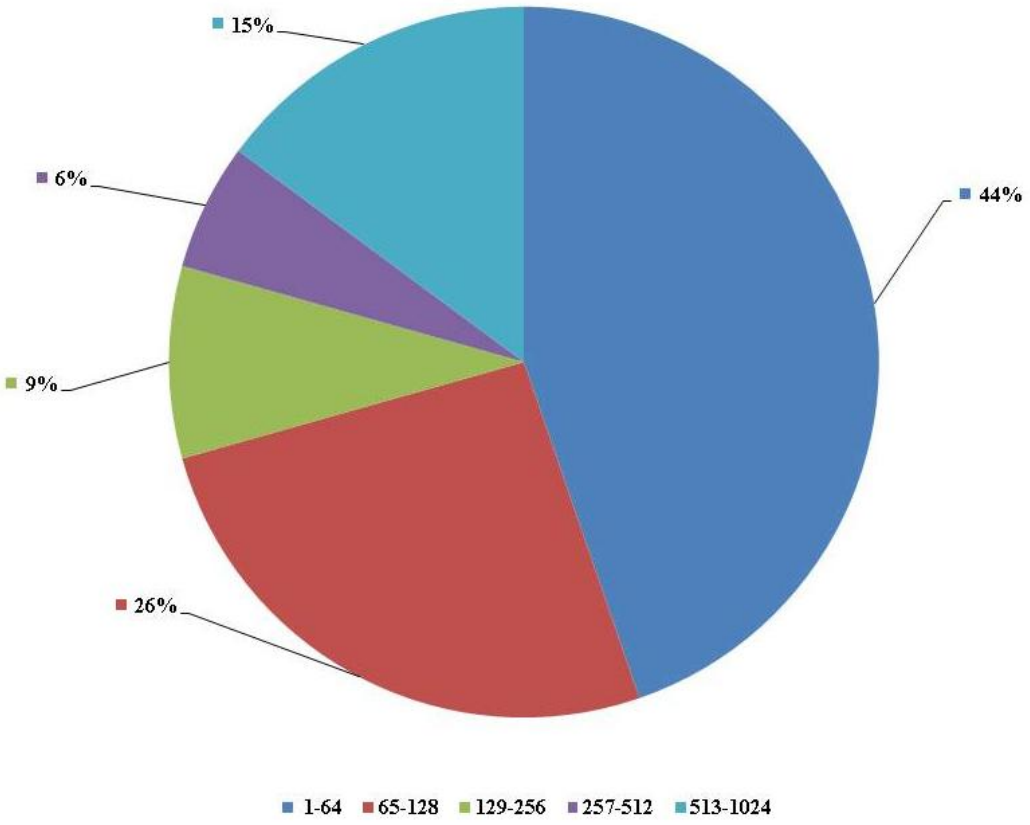
Job Queues: Idle Jobs - Jobs waiting in queue to start running



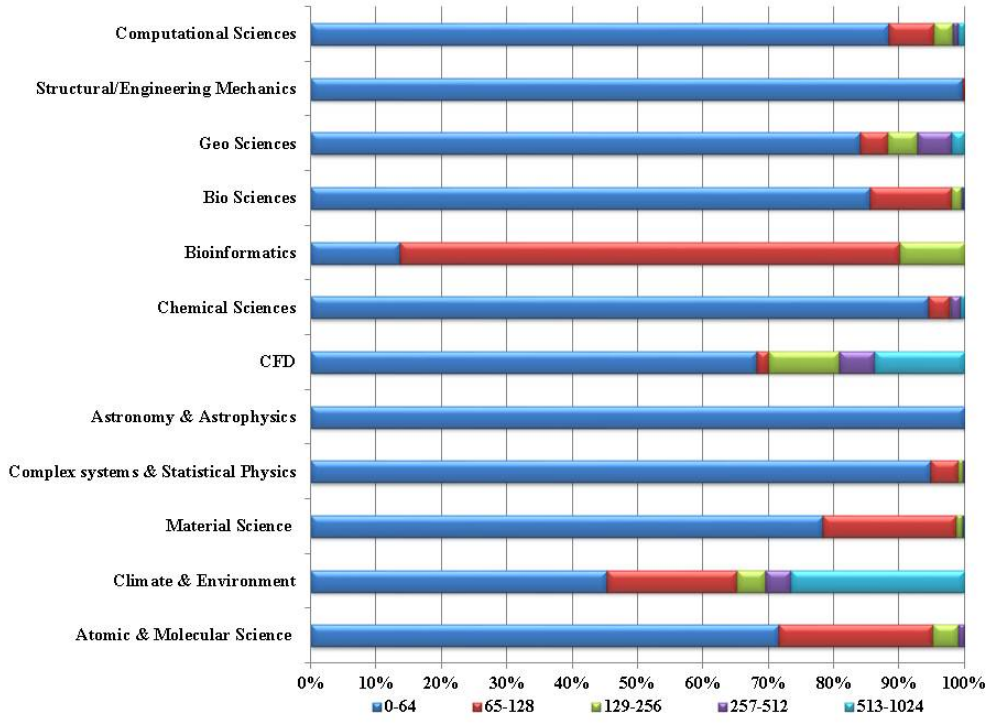
From the figures above, we see that about 100 jobs are running and equal number of jobs are always in queue waiting for their turn to start running. This indicates the need for more resources.

CPU Utilization (Period: Apr. 1, 2014 - Mar. 15, 2015)

CPU Time utilization vs no. of cores

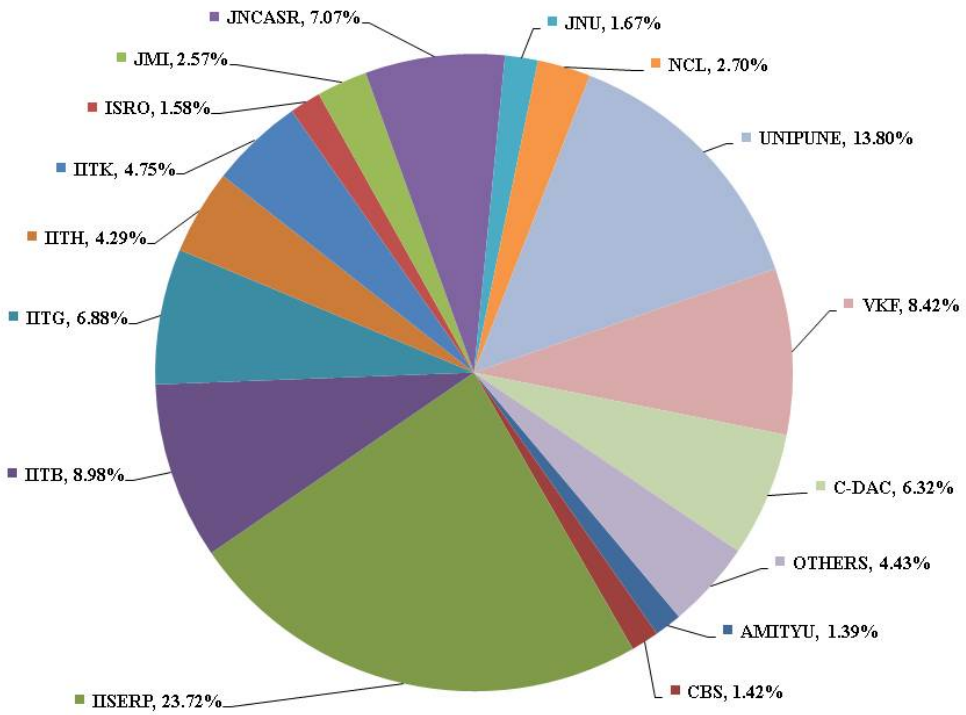


Job Size (CPU cores) across application domains

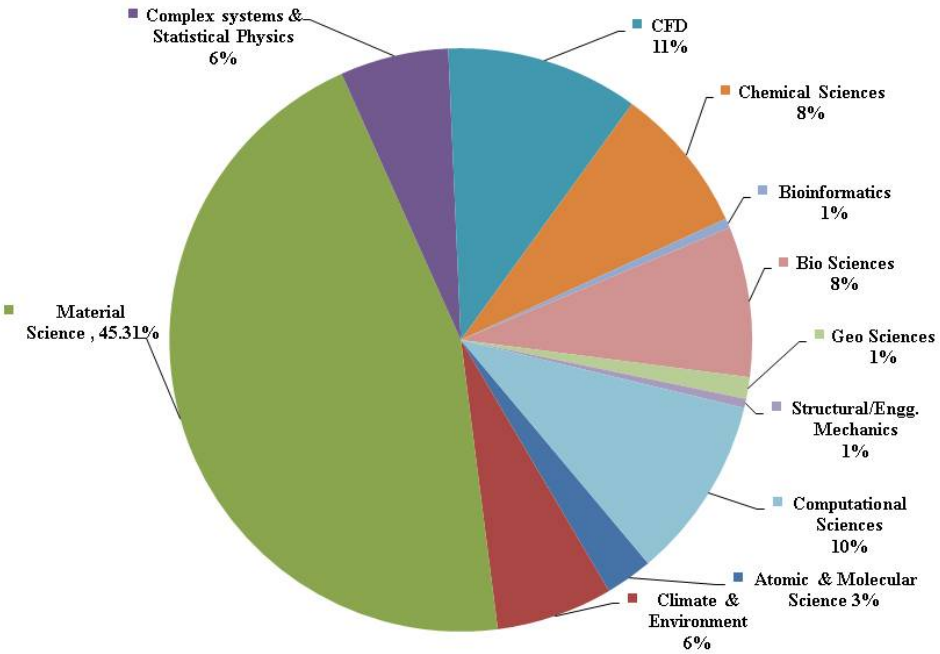


CPU Utilization (Period: Apr. 1, 2014 - Mar. 15, 2015)

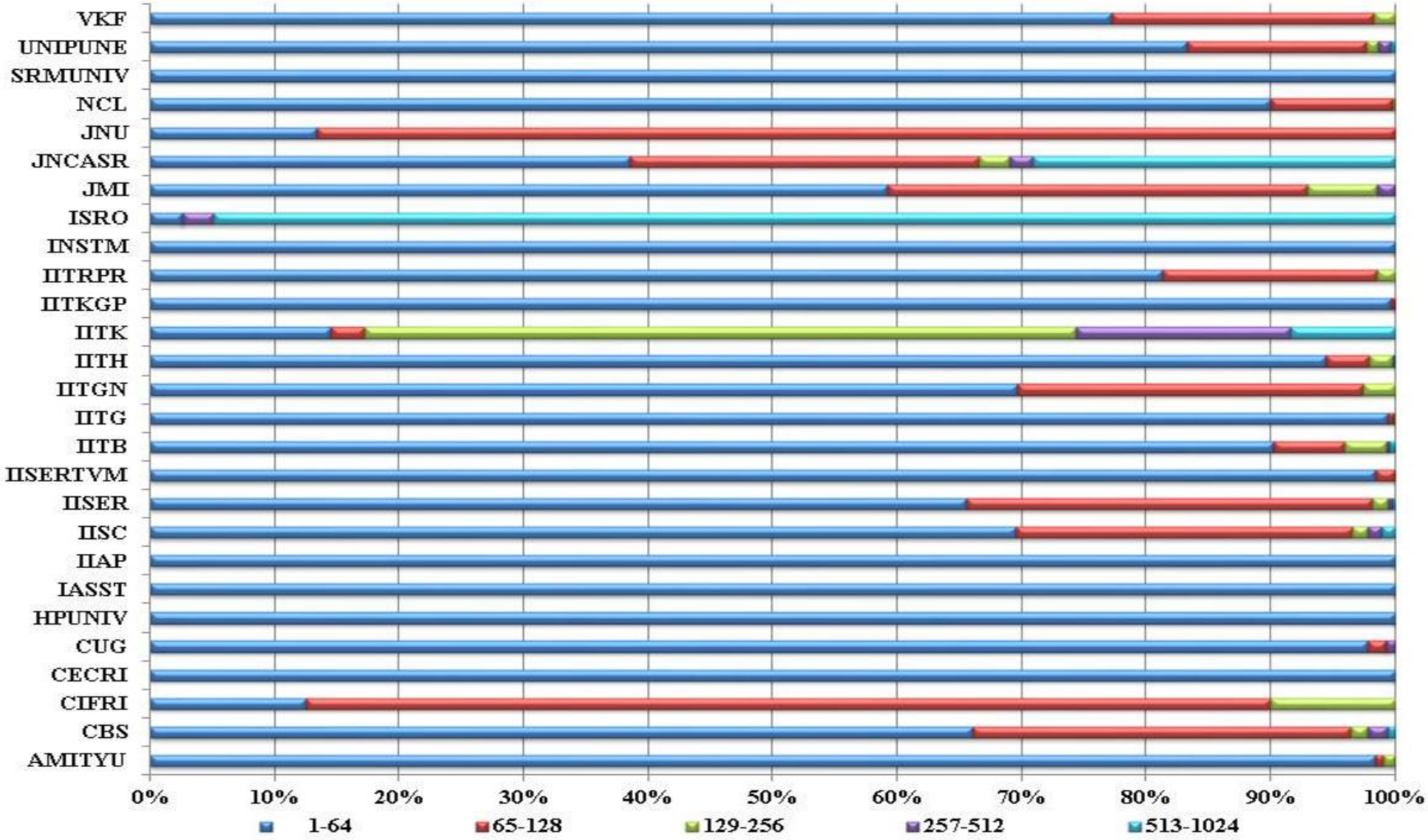
Institute wise CPU utilization in (%)



CPU time utilization in (%) across application domains



Job Statistics (Period: Apr. 1, 2014 - Mar. 15, 2015)



Job Size (CPU cores) across Institutions
(*External users*)

All Users:

Number of Jobs = 54673 (Period: Apr. 1, 2014 - Mar. 15, 2015)

Total Number of Jobs = 142420 (Period: Feb. 19, 2013 - Mar. 15, 2015)

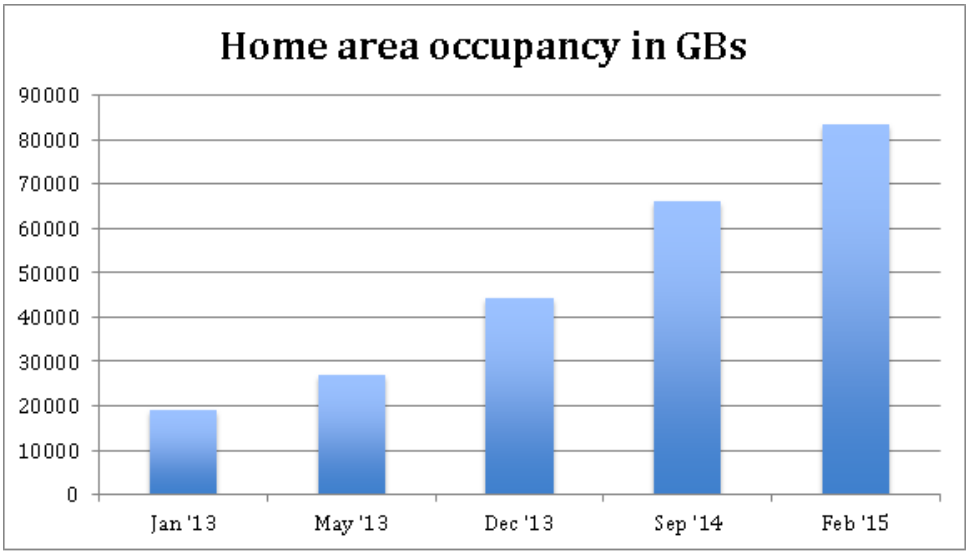
Jobs across Domains

Table 6.2: Jobs across Domains

Domain	Jobs
Atomic & Mol. Sc	405
Bioinformatics	81
Bio Science	3487
CFD	1748
Climate & Environment	5310
Complex System	2164
Chemical Science	3004
Geo Sciences	2227
Material Science	24754
Structural/ Eng. Mechanics	1312
Others (Comput. Sc.)	10181
Total	54673

Storage usage statistics:

The statistics of the storage on PARAM Yuva II is summarized in the table below. The statistics of the /home area occupancy, the change in the size of the data stored and the change in the number of files are shown in the plots below.

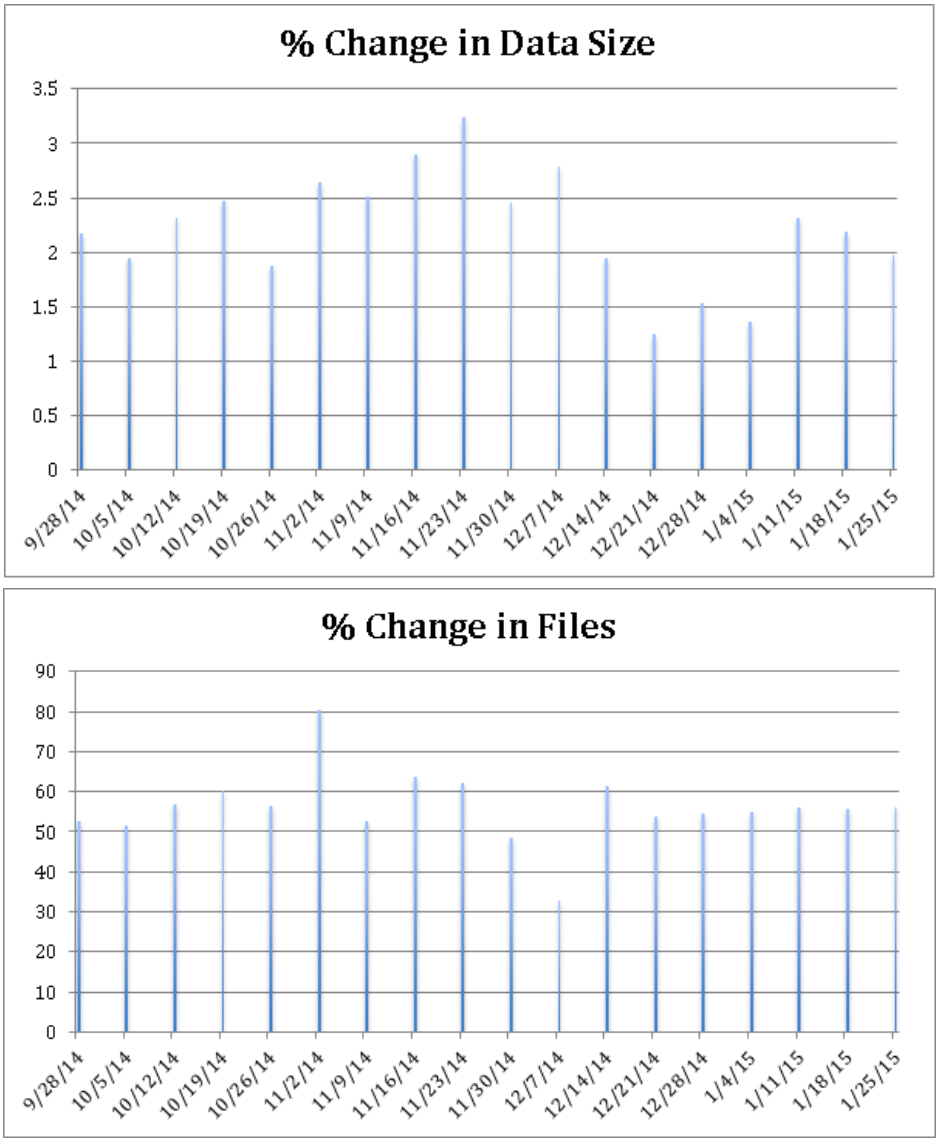


Every user of PARAM YuvaII has a storage quota allocated. Total of such quota allocations has reached 182.78 TB which is 96.2 % of the available storage space. Besides this an additional quota is allocated to user as per the request for a fixed short durations. Also it

is to be noted that 80% of the total number of files are small files, however it is the larege files which constitutes the majority of the storage capacity usage. It is to be noted that the storage is divided into home area and high performance scratch area as mentioned in the compute resources. It has been observed that about 822 jobs have used the *scratch area available for data staging.*

Table 6.3: Variation of /home area in the storage.

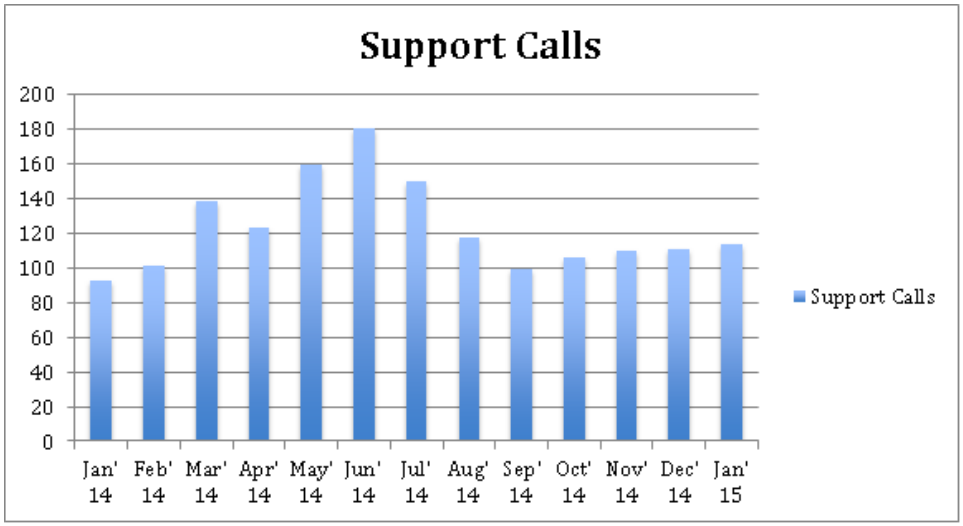
Date	Size (in TB)	No. of files
13 Sep. 2014	66.2	73,81,852
15 Feb. 2015	82.0	14,35,79,981



User Support Calls:

The NPSF-Help team handles about 120 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.



7

Dedicated Slot Booking Facility

The Dedicated Slot Booking Facility (DSBF) was introduced for the users to offer better quality of service over and above the usual batch processing system. This facility helps the users *to plan their computing exercises over an extended period of time* as the compute resources are committed for their jobs during these slots. This comes with the advantage of not having to wait for the jobs to start as in the batch queue as long as they have not exhausted the resources committed to them. The primary aim of this scheme is to encourage users towards *capability computing* and *scaling exercise* of their applications, keeping in mind the preparedness required for the Peta scale computing era. However, at present the users are permitted to run a large number of small jobs (capacity computing) also towards the efficient utilization of their slots.

Under this scheme, the users can book a slot[¶] for a maximum of 15 days, requesting for resources up to 64 nodes[‖]. These dedicated slots are announced periodically and the slot booking facility is made available through NPSF portal `https://npsf.cdac.in`. The users can book the slots on first come, first serve basis. The *eligibility criteria for booking the slot* is specified in the announcement of the slot booking in order to *ensure fairness across the user community in availing the slots* under DSBF. The users are expected to submit a report of the utilization of the slot and the activity carried out in the given format.

Apart from this, there are slots available (*in chunks for a duration of less than 24 hrs*) with compute resources of 64 nodes on consecutive days starting from a particular date and time for a specified period of time. These slots could be used for running jobs with checkpoint enabled applications in order to restart the interupted job at a later point of time. The request for immediate resources from users were accomodated in these slots on a case to case basis as per the requirement. In the due course of time, several of the users have confided that they would be able to use these slots effectively for their jobs. In view of this, these slots were also brought under the purview of DSBF recently and the booking is handled through the portal now.

The table[**] below gives a summary of the slots under DSBF during 2014-15. The summary of the usage of the slots prior to April 2014 is given in Appendix B.

[¶]The duration of the slot is given in dd:hh:mm:ss format.

[‖]1 node = 16 CPU cores.

[**]The users are mapped to project(s) and every project has a Chief Investigator and the CPU time is credited to/debited from their respective project account. This applies to CPU utilization for the jobs through batch processing as well as DSBF.

Table 7.1: Summary of the utililiztion of dedicated slots

User	Chief Investigator	Institution	Domain	Start Time	Duration	# Nodes
2015						
Dr. Kavita Joshi	Dr. Kavita Joshi	NCL Pune	Chemical Sc.	2015-03-16 01:01:00.0	1:0:0:00	64
Ms. Anju Susan	Dr. Kavita Joshi	NCL Pune	Chemical Sc.	2015-03-13 01:01:00.0	2:0:0:00	16
Ms. Nalini Gurav	Dr. Rajeev Pathak	UniPune	Complex Syst.	2015-03-12 12:01:00.0	2:0:0:00	24
Mr. Vaibhav Kaware	Dr. Kavita Joshi	NCL Pune	Chemical Sc.	2015-03-12 01:01:00.0	2:0:0:00	8
Ms. Deepika Goyal	Prof. Rakesh Kumar	IIT Ropar	Material Sc.	2015-03-12 01:01:00.0	1:0:0:00	16
Dr. Ashutosh Kumar	Prof. A. Bhattacharya	IIT Bombay	Bio Sc.	2015-03-11 18:01:00.0	3:0:0:00	16
Dr. Pradeep Kumar	Prof. A. Bhattacharya	IIT Bombay	Chemical Sc.	2015-03-11 01:01:00.0	1:0:0:00	8
Mr. Reman Singh	Dr. Arnab Mukharjee	IISER Pune	Complex Syst.	2015-02-25 1:01:00:00	14:0:0:00	64
Mr. Debasis Saha	Dr. Arnab Mukherjee	IISER Pune	Complex Syst.	2015-02-23 10:01:00:00	1:0:0:00	64
Mr. Mit Naik	Dr. Manish Jain	IISc Bangalore	Material Sc.	2015-02-22 1:01:00:00	1:0:0:00	64
Mr. Manjunatha V	Mr. Prashant Dinde	C-DAC	Comput. Sc	2015-02-20 09:00:00:0	0:9:0:00	8
Mr. Manjunatha V	Mr. Prashant Dinde	C-DAC	Comput. Sc	2015-02-19 09:00:00:0	0:9:0:00	8
Dr. Mrinalini Deshpande	Dr. Mrinalini Deshpande	HPT Arts & RYK Sc. Coll., Nasik	Material Sc.	2015-02-17 12:01:00:00	4:0:0:00	64
Mr. Sagar Khavnekar	Dr. Avinash Kale	CBS Mumbai	Bio Sc.	2015-02-16 00:01:00:00	0:12:00:00	64
Mr. Nandha Kumar	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2015-02-01 1:01:00:00	14:23:0:00	64
Mr. Sagar Khavnekar	Dr. Avinash Kale	CBS mumbai	Bio Sc.	2015-01-31 01:01:00.0	1:00:0:00	64
Mr. Saurabh Gupta	Prof. A. Bhattacharya	IIT Bombay	Comput. Sc.	2015-01-29 01:01:00.0	2:0:0:00	64
Mr. Sagar Khavnekar	Dr. Avinash Kale	CBS Mumbai	Bio Sc.	2015-01-23 11:00:00.0	5:14:0:00	48
Dr. Rakesh Kumar	Dr. Rakesh Kumar	IIT Ropar	Material Sc.	2015-01-23 11:00:00.0	5:14:0:00	16
Mr. Sagar Khavnekar	Dr. Avinash Kale	CBS Mumbai	Bio Sc.	2015-01-15 01:01:00.0	8:10:0:00	64
Ms. V. M. Hridya	Dr. Arnab Mukherjee	IISER Pune	Complex Syst.	2015-01-14 01:01:00.0	1:0:0:00	40
Mr. Rohit Babar	Dr. Mukul Kabir	IISER Pune	Material Sc.	2015-01-02 01:01:00.0	10:0:0:00	32
Dr. R. Thenmalarchelvi	Dr. R. Thenmalarchelvi	IIT Hyderabad	Bio Sc.	2015-03-09 17:00:00.0	††7:0:0:0	64
Dr. Bheema Lingam C	Prof. Vijay Kumar	VKF Gurgaon	Material Sc.	2015-03-02 17:00:00.0	††7:0:0:0	64

Continued on next page

Table 7.1 – *Continued from previous page*

User	Chief Investigator	Institution	Domain	Start Time	Duration	# Nodes
Mr. Bappa Ghosh	Dr. Srabanti Chaudhury	IISER Pune	Bio Sc.	2015-02-23 17:00:00.0	††7:0:0:0	64
Dr. Ambarish Kunwar	Prof. A Bhattacharya	IIT Bombay	Comput. Sc.	2015-02-16 17:00:00.0	††7:0:0:0	64
Mr. Praveen kumar	Dr. Arun Venkatnathan	IISER Pune	Chemical Sc.	2015-02-09 17:00:00.0	††7:0:0:0	64
Dr. Souvik Paul	Prof. Subhradip Ghosh	IIT Guwahati	Material Sc.	2015-02-02 17:00:00.0	††7:0:0:0	64
Ms. Vasundhara Shewale	Dr Mrinalini Deshpande	HPT Arts & RYK Sc. Coll., Nasik	Material Sc.	2015-01-26 17:00:00.0	††7:0:0:0	64
Dr. Mukul Kabir	Dr. Mukul Kabir	IISER Pune	Material Sc.	2015-01-19 17:00:00.0	††7:0:0:00	64
Ms. Niharika Joshi	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2015-01-12 17:00:00.0	††7:0:0:00	64
Mr. Subrahmanyam S	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2015-01-05 17:00:00.0	††7:0:0:00	64
2014						
Dr. Amol B. Rahane	Prof. Vijay Kumar	VKF Gurgoan	Material Sc.	2014-12-30 11:01:00.0	14:0:0:00	32
Ms. Sanjana Nair	Dr. R. Thenmalarchelvi	IIT Hyderabad	Bio Sc.	2014-12-30 11:01:00.0	2:0:0:00	32
Mr. Debashish Das	Prof. Subhradip Ghosh	IIT Guwahati	Material Sc.	2014-12-29 01:01:00.0	1:0:0:00	16
Ms. Arra Srilatha	Dr. Mukul Kabir	IISER Pune	Material Sc.	2014-12-23 01:01:00.0	6:0:0:00	12
Mr. Souvik Paul	Prof. Subhradip Ghosh	IIT Guwahati	Material Sc.	2014-12-22 13:01:00.0	7:0:0:00	16
Dr. Santosh Kulkarni	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2014-12-15 12:01:00.0	14:0:0:00	32
Mr. Rohit Babar	Dr. Mukul Kabir	IISER Pune	Material Sc.	2014-12-15 11:01:00.0	7:0:0:00	32
Mr. Nandha Kumar	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2014-12-01 01:01:00.0	14:0:0:00	64
Ms. Sanjana Nair	Dr. R. Thenmalarchelvi	IIT Hyderabad	Bio Sc.	2014-11-29 11:01:00.0	1:0:0:00	64
Mr. Mandar Kulkarni	Dr. Arnab Mukherjee	IISER Pune	Bio Sc.	2014-11-15 10:01:00.0	14:0:0:00	64
Prof. Mahendra Verma	Prof. Mahendra Verma	IIT Kanpur	CFD	2014-07-16 11:00:00:0	10:0:0:00	64
Prof. Shridhar Gadre	Prof. Shridhar Gadre	IIT Kanpur	Chemical Sc.	2014-07-01 11:00:00:0	15:00:00:0	64
Mr. Shailesh Pandey	Prof. Indira Ghosh	JNU	Bio Sc.	2014-06-22 11:00:00:0	09:00:00:0	64
Mr. Abhishek Shrivastav	Ms. Richa Rastogi	C-DAC	Geo Sc.	2014-06-07 11:00:00:0	14:23:59:00	64
Dr. Amol B. Rahane	Prof. Vijay Kumar	VKF Gurgoan	Material Sc.	2014-06-04 11:00:00:0	3:0:0:00	64
Dr. R. Thenmalarchelvi	Dr. R. Thenmalarchelvi	IIT Hyderabad	Bio Sc.	2014-05-22 11:00:00:0	14:0:0:00	64
Mr. Saurabh Gupta	Prof. A. Bhattacharya	IIT Bombay	Comput. Sc.	2014-04-17 01:01:00.0	1:0:0:00	64
Dr. Kavita Joshi	Dr. Kavita Joshi	NCL Pune	Chemical Sc.	2014-04-01 11:01:00.0	14:23:59:00	64

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Table 7.1 – *Continued from previous page*

User	Chief Investigator	Institution	Domain	Start Time	Duration	# Nodes
Mr. Aditya Gupte	Prof A. Bhattacharya	IIT Bombay	CFD	2014-12-30 17:00:00:0	††6:0:0:00	64
Ms. Priya Francis	Dr. S. V. Ghaisas	UniPune	Material Sc.	2014-12-25 17:00:00:0	††5:0:0:00	64
Mr. Prasenjit Ghosh	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2014-12-18 17:00:00:0	††7:0:0:00	64
Ms. Priya Francis	Dr. S. V. Ghaisas	UniPune	Material Sc.	2014-11-19 17:00:00:0	††7:0:0:00	64
Dr. R. Thenmalarchelvi	Dr. R. Thenmalarchelvi	IIT Hyderabad	Bio Sc.	2014-11-12 17:00:00:0	††7:0:0:00	64
Ms. Priya Francis	Dr. S. V. Ghaisas	UniPune	Material Sc.	2014-11-10 17:00:00:0	††4:9:0:00	54
Prof. Mahendra Verma	Prof. Mahendra Verma	IIT Kanpur	CFD	2014-09-23 17:00:00:0	††50:0:0:0	64
Dr. Prasanth P	Prof. Roddam Narasimha	JNCASR	CFD	2014-05-17 17:00:00:0	††121:0:0:0	64
Dr. Prasanth P	Prof. Roddam Narasimha	JNCASR	CFD	2014-04-10 17:00:00:0	††20:0:0:00	64
Dr. Prasanth P	Prof. Roddam Narasimha	JNCASR	CFD	2014-04-03 17:00:00:0	††2:0:0:00	64

††These slots are in chunks (of 16 hrs 55 min duration) available for consecutive days.

8

Major Research Projects

This is the list of projects[‡‡] based on the compute time usage and research publications in high impact journals from the work that is carried out on PARAM Yuva II.

First principles static, dynamic and electronic properties of Liquid Metal Alloys
Prof. Pradeep K. Ahluwalia, Himachal Pradesh University, Shimla

Theoretical study of structural, electronic and magnetic properties of nanomaterials
Dr. Mrinalini Deshpande, HPT Arts and RYK Science College, Nasik

Defects in Oxides
Dr. Manish Jain, IISc, Bangalore

Multiscale simulation of shear of miceller systems
Dr. Apratim Chatterji, IISER, Pune

Molecular modelling and dynamics of polymers, gas hydrates and ionic liquids: An alternative energy initiative
Prof. Arun Venkatnathan, IISER, Pune

Materials modelling at different length and time scales
Dr. Mukul Kabir, IISER, Pune

Study of CdS and CdTeS quantum dots decorated on TiO_2 nanowires
Dr. Prasenjit Ghosh, IISER, Pune

High Performance Computing initiative (IIT, Bombay)
Prof. Jhumpa Adhikari (Chemical Engg.), Prof. P. I. Pradeepkumar (Chemistry)

First principles based investigations of shape memory alloys and oxide multiferroics
Prof. Subhradip Ghosh, IIT, Guwahati

[‡‡]Please refer Appendix A for the complete list of projects.

Hydrophobic interactions in different chemical environment
Dr. Sandip Paul, IIT, Guwahati

First principles studies on optical, geophysical and superconducting materials
Dr. V. Kanchana, IIT, Hyderabad

Structure and dynamics of RMA duplexes comprising of trinucleotide repeat expansion
Dr. Thenmalarchelvi Rathinavelan, IIT, Hyderabad

Magnetohydrodynamics turbulance studies of liquid metals and dynamo
Prof. Mahendra K. Verma, IIT, Kanpur

Molecular Tailoring Approach: Ab-initio treatment of large molecules and molecular clusters
Prof. Shridhar R. Gadre, IIT, Kanpur

Study of effects of point mutations on the conformational dynamics
Dr. Neelanjana Sengupta, NCL, Pune

The study of diffusion coefficient of Te on Cd-Te surface(111)
Mr. Ebadollah Naderi, S. P. Pune University

9

Ph.D Theses by PARAM Yuva II users

Number of Ph.D theses in 2014-15 : 3

1. **Electronic structure characterization of molecular interactions in clathrate hydrates** (June, 2014)
   Student: Ms. K. R. Ramya, Dept. of Chemistry, IISER, Pune
   Supervisor: Prof. Arun Venkatanathan

2. **First-principles electronic structure based investigations of Mn_2NiX magnetic alloys with Inverse Heusler structure** (August, 2014)
   Student: Mr. Souvik Paul, Dept. of Physics, IIT, Guwahati
   Supervisor: Prof. Subhradip Ghosh

3. **Anisotropic energy spectrum, flux and transfers in quasi-static magnetohydrodynamic turbulence** (September, 2014)
   Student: Mr. K. Sandeep Reddy, Dept. of Physics, IIT, Kanpur
   Supervisor: Prof. Mahendra K. Verma

Number of Ph.Ds produced: 10
(Please refer Appendix(C) for Ph.D theses prior to 2014-15.)

10

Science using PARAM Yuva II

Publications by NPSF users

Total no. of Publications: 24

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. Journals with higher impact factors are deemed to be more important than those with lower ones.

ACS Chemical Biology (5.356)

V. Dhamodharan, S. Harikrishna, A. C. Bhasikuttan, and P. I. Pradeepkumar, Topology specific stabilization of promoter over telomeric quadruplex DNAs by bisbenzimidazole carboxamide derivatives, ACS Chem. Bio. (2015). (*Accepted*)

PLoS Computational Biology (4.829)

N. Khan, T. Rathinavelan, and N. Kolimi, Twisting Right To Left: A Mismatch In A CAG Trinucleotide Repeat Overexpansion Provokes Left-Handed Z-DNA Conformation, PLoS Comput. Biol. (2015). (*Accepted*)

Journal of Physical Chemistry C (4.814)

Leena George, Subrahmanyam Sappati, Prasenjit Ghosh, R. Nandini Devi, Surface Site Modulations by Conjugated Organic Molecules to Enhance Visible Light Ativity of ZnO Nanostructures in Photocatalytic Water Splitting, J. Phys. Chem. C (2015). (*Accepted*)

Aakanksha Chaudhary, M. Poshit Nag, N. Ravishankar, Tiju Thomas, Manish Jain, and Srinivasan Raghavan, Synergistic Effect of Mo + Cu Codoping on the Photocatalytic Behavior of Metastable TiO_2 Solid Solutions, J. Phys. Chem. C **118**, 29788 (2014).

Journal of Physical Chemistry B (4.189)

Shubhadip Das and Sandip Paul, Exploring Molecular Insights into Aggregation of Hydrotrope Sodium Cumene Sulfonate in Aqueous Solution: A Molecular Dynamics Simulation Study, J.Phys. Chem. B. **119**, 3142 (2015).

K. R. Ramya, Praveen Kumar, Ashish Kumar, and A. Venkatnathan, Interplay of Phase Separation, Tail Aggregation, and Micelle Formation in the Nanostructured Organization of Hydrated Imidazolium Ionic Liquid, J. Phys. Chem. B. **118**, 8839 (2014).

Physical Review B (3.767)

M. Kabir and T. Saha-Dasgupta, Manipulation of edge magnetism in hexagonal graphene nanoflakes, Phys. Rev. B **90**, 035403 (2014).

PLoS ONE (3.73)

P. Chatterjee, Jaya C. Jose, N. Sengupta, Cross Dimerization of Amyloid-β and αSynuclein Proteins in Aqueous Environment: A Molecular Dynamics Simulations Study, PLoS ONE, **9**, e106883 (2014).

RSC Advances (3.708)

Subrata Paul and Sandip Paul, Effects of the temperature and trehalose concentration on the hydrophobic interactions of a small nonpolar neopentane solute: a molecular dynamics simulation study, RSC Advances **4**, 34267 (2014).

Brij Mohan, Ashok Kumar and P. K. Ahluwalia, Electronic and Dielectric Properties of Silicene Functionalized with Monomers, Dimers and Trimers of B, C and N atoms, RSC Advances **4**, 31700 (2014).

M. More, A. P. Sunda, and A. Venkatnathan, Polymer chain length, phosphoric acid doping and temperature dependence on structure and dynamics of ABPBI [poly(2,5-benzimidazole)] polymer electrolyte membrane, RSC Advances **4**, 19746 (2014).

Journal of Chemical Physics (3.164)

N. Sahu and S. R. Gadre, Accurate vibrational spectra via molecular tailoring approach: A case study of water clusters at MP2 level, J. Chem. Phys **142**, 014107 (2015).

Journal of Physics: Condensed Matter (2.355)

S. Paul, B. Sanyal and S. Ghosh, First-principles study of the lattice instabilities in Mn_2NiX (X=Al, Ga, In, Sn) magnetic shape memory alloys, J. Phys.: Condensed Matter **27**, 035401 (2015).

Physical Review E (2.313)

Shaikh Mubeena and Apratim Chatterji, Hierarchical self-assembly: Self-organized nanostructures in a nematically ordered matrix of self-assembled polymeric chains, Phys. Rev. E (2015). (*Accepted*)

A. Kumar, A. G. Chatterjee, and M. K. Verma, Energy spectrum of buoyancy-driven turbulence Energy spectrum of buoyancy-driven turbulence, Phys. Rev. E **90**, 023016 (2014).

S. Bhaumik and T. K. Sengupta, Precursor of transition to turbulence: Spatiotemporal wave front, Phys. Rev. E **89**, 043018 (2014).

Journal of Applied Physics (2.185)

S. Paul, A. Kundu, B. Sanyal and S. Ghosh, Anti-site disorder and improved functionality of Mn_2NiX (X = Al, Ga, In, Sn) inverse Heusler alloys, J. Appl. Phys. **116**, 133903 (2014).

G. Shwetha, V. Kanchana, M. C. Valsakumar, Excitonic effects in oxyhalide scintillating host compounds, J. Appl. Phys. **116**, 133510 (2014).

Journal of Chemical and Engineering Data (2.045)

M. Harini, Jhumpa Adhikari, and K. Yamuna Rani, Prediction of Vapor Liquid Coexistence Data for p-Cymene Using Equation of State Methods and Monte Carlo Simulations, Journal of Chemical & Engineering Data **59**, 2987 (2014).

AIP Advances (1.59)

Ebadollah Naderi, Sachin Nanavati, Chiranjib Majumder, and S. V. Ghaisas, Diffusion of Cd and Te adatoms on CdTe(111) surfaces: A computational study using density functional theory, AIP Advances **5**, 017134 (2015).

Physica E (1.522)

Brij Mohan, Ashok Kumar, and P. K. Ahluwalia, Electronic and Optical Properties of Silicene Under Uni-axial and Bi-axial Mechanical Strain: A First Principle Study, Physica E **61**, 40 (2014).

Computational and Theoretical Chemistry (1.371)

Sandip Kumavat, Mrinalini Deshpande, Alkali Metal Doped Nickel Oxide Clusters: A Density Functional Study, Computational and Theoretical Chemistry **1035**, 19 (2014).

Journal of Nanostructure in Chemistry

S. Chopra and B. Rai, DFT/TDDFT study of electronic and optical properties of Surface-passivated Silicon nanocrystals, Si_n ($n = 20, 24, 26$ and 28), J. of Nanostructure in Chemistry (2015). (*Accepted*) http://dx.doi.org/10.1007/s40097-015-0150-5

Preprint

Neha V. Karanjkar and Madhav P. Desai, Optimization of Discrete-parameter Multiprocessor Systems using a Novel Ergodic Interpolation Technique, arXiv:1411.2222 [cs.DC].

11

Workshops organized/participated

NPSF has been involved with several activities towards HPC proliferation and academic outreach programmes along with the primary task of facility management and user support. The workshops conducted before April 2014 are listed in Appendix D. The activities during the year 2014-15 are listed below:

1. Lectures in the **HPC workshop** for *Ghana participants*, organized by High Performance Computing Solutions group of C-DAC, Pune on Aug. 11-12, 2014. The lectures delivered were:

   i. Unconventional Computing by Dr. Sandeep K. Joshi

   ii. Changing Trends in Scientific Computing: Are we ready? by Dr. V. Venkatesh Shenoi

   iii. Energy Efficient HPC by Mr. Rishi Pathak

   The visit to the PARAM Yuva II facility for the workshop participants was facilitated by Mr. Maneesh Kumar for the partipants of this workshop.

2. Organized the workshop on **Scientific Applications on PARAM Yuva II** on Jan. 8-9, 2015 at Indian Institute of Tropical Meteorology (IITM), Pune.

   The workshop was organized by NPSF to commemorate successful completion of two (2) years of commissioning of PARAM Yuva II. The objective of the workshop was to *share the experiences of users and highlight their research work* using PARAM Yuva I I. It also provided an opportunity for interaction and knowledge sharing among users from different scientific domains.

   Shri Sanjay Wandhekar, Associate Director & H.O.D., NPSF welcomed the participants of the workshop. The workshop was graced by the presence of Dr. R. Krishnan, Director (Act.), IITM and Dr. Hemant Darbari, Executive Director, C-DAC, Pune. Dr. Hemant Darbari gave the welcome address and talked about the challenges ahead in HPC. The keynote talk on "Foretelling the monsoon" was delivered by Prof. Sulochana Gadgil from Centre for Atmospheric and Oceanic Sciences (CAOS), IISc, Bangalore. Prof. Gadgil highlighted the importance of High Performance Computing (HPC) in paving the way for more and more accurate numerical weather predictions.

Diginataries on the dais during the inauguration of the workshop.

The workshop witnessed the participation of around 124 participants. The first day of the workshop had talks of broader interest from various domains. There were around 10 talks including presentations from NPSF members covering topics like the PARAM Yuva II Ecosystem, Performance analysis tools, Programming models, Trends in GPU Computing and Exascale challenges. The second day of the workshop had two parallel sessions: (1) Material Science & Bio Science and (2) Chemical Science & Engineering Sciences (covering CFD, Climate Science, Geo Science and Structural Mechanics). There were around 27 talks spread across these two parallel sessions.

Welcome address by Dr. Hemant Darbari, Executive Director, C-DAC, Pune.

The invited talks were delivered by faculty and student speakers on the scientific research they pursued covering how their research work leveraged HPC and PARAM Yuva II. The workshop also involved talks from C-DAC members about the work done on PARAM Yuva II in application areas like Climate Science, Computational Fluid Dynamics, Material Science, Chemical Science, Geo Science, Structural Mechanics, Biophysics and Bioinformatics.

Prof. Sulochana Gadgil delivering the keynote address in the workshop.

The proceedings of the workshop was also made available *live on both days through in-house conducted webinar* for the PARAM Yuva II users. The option was made available to join any of the parallel sessions scheduled on the second day, i.e. on Jan. 9, 2015. *About forty (40) users from remote locations participated in the workshop through this webinar.*

The workshop concluded with deliberating on few of the suggestions that came from the participants. The final vote of thanks was given by Dr. Sandeep K. Joshi, Principal Technical Officer, NPSF.

Note: Some more picures of the workshop are available in the picture gallery section.

12

PARAM Yuva II Visits

Visits by Officials, Members of Academia & Industry

1. Shri. R. S. Sharma, Honourable Secretary, DeitY, GoI (Oct. 10, 2014).
2. Prof. Yutaka Ishikawa, University of Tokyo (Dec. 21, 2014).
3. Mr. Tony Kingsmith, Executive Vice President (Marketing), Imagination Technologies (Jan. 21, 2015).
4. Shri. Tripurari Sharan, Principal Secretary, Dept. of IT & Dept. of Agriculture, Governemt of Bihar (Jan. 30, 2015).
5. Shri Revana Siddeshwar, Chief Manager, ITI Limited (Feb. 10 , 2015).
6. Shri. Kumar Tuhin, Joint Secretary, Development Partnership Administration, Ministry of External Affairs, GoI (Feb. 11, 2015).
7. Lt. Cdr. Sundar, INMAC and Lt. Cdr. Manoj K. Mahauar, NODPAC, Indian Navy, Kochi (Feb. 17, 2015).
8. Mr. R. M. Math (ED) and Mr. Sachin Waingankar (Head-Solutions), CNRVGD Tech (Mar. 2, 2015).

Visits as part of various programmes

1. Major General R. P. Bhadran & IPMT team (Aug. 19, 2014).
2. Delegation of Japanese corporate trainees from Softbridge Solutions (Aug. 22, 2014).
3. C-DAC Induction Programme (Oct. 11, 2014).
4. Participants (25) of the Indo-Russian workshop on **High Performance Computing for Computer Aided Engineering & Sciences**, Nov. 18-20, 2014 (Nov. 19, 2014).
5. Participants and delegates of **IEEE Indicon 2014** (Dec. 13, 2014).
6. Participants (75) of **Accelerating Biology 2015** organized by Bioinformatics group, C-DAC, Pune, Jan. 20-22 (Jan. 20, 2015).
7. Participants (21) of **Manager's Development Programme** organized by C-DAC, Pune (Feb. 9, 2015).

8. Participants (35 members, including Officers and Cadets) of the Mid-term hike of Officers Training Academy, Gaya (Mar. 17, 2015).

Industrial Visits for students

The students of CGPIT, Surat on Dec. 12, 2014 during the presentation.

Table 12.1: Summary of Industrial Visits for students

Institution	No. of visitors	Visit Date
2014		
Department of Commerce and Research Centre, UniPune	30	Apr. 07
NIT Silchar	30	Jun. 02
Engineering College,	60	Jul. 08
Indo-Ghana Centre for Excellence	8	Aug. 12
Techno India NJR Institute of Technology, Udaipur	56	Aug. 19
Sabu Siddiqui College of Engineering, Mumbai	60	Aug. 21
Deepstambh Foundation, Jalgaon	40	Aug. 21
SVERI's College of Engineering, Pandharpur	60	Sep. 01
ISSC, UniPune	32	Sep. 11
Rajiv Gandhi Institute of Technology, Mumbai	100	Sep. 12
St. Francis College, Mumbai	100	Sep. 15
Army Institute of Technology, Pune	43	Sep. 25
G. V. Acharya College of Polytechnic, Shelu, Raigad	60	Sep. 26
M. J. College, Bhilai	16	Oct. 10
St. Xavier's College, Mumbai	55	Oct. 13
College of Engineering, Pune	38	Oct. 16
Akbar Peerbhoy College of Commerce & Economics	100	Dec. 09
Computer and Information Technology Board, SPPU	20	Dec. 11

Continued on next page

Table 12.1 – *Continued from previous page*

Institution	No. of visitors	Visit Date
Chhotubhai Gopalbhai Patel Institute of Technology, Surat	120	Dec. 12
Sant Rawool Maharaj Mahavidyalaya, Kudal, Dt. Sindhudurg, Maharashtra	68	Dec. 17
M. H. Saboo Siddik Polytechnic, Mumbai	64	Dec. 30
2015		
Bharati Vidyapeeth, Pune	34	Jan. 15
B. D. Kale Mahavidyalaya, Ghodegaon	55	Jan. 19
Mahatma Gandhi Mission Dr. G. Y. P. College of Comp. Sc. & IT, Aurangabad	55	Jan. 21
Deogiri College, Aurangabad	55	Feb. 03
Latthe Polytechnic, Sangli	24	Feb. 06
Don Bosco Institute of Technology, Mumbai	52	Feb. 09
Arts, Science and Commerce College, Rahuri, Ahmednagar	40	Feb. 06
Pune Institute of Computer Technology, Pune	100	Feb. 10
Yashwantrao Chavan Institute of Rural Development, Shivaji University, Kolhapur	22	Feb. 11
Pune Institute of Computer Technology, Pune	37	Feb. 24
Prahladrai Dalmia Lions College of Commerce and Economics	53	Feb. 27
VAMNICOM, Pune	18	Feb. 27
D. Y. Patil Polytechnic, Talsande, Kolhapur	37	Feb. 28
PUMBA, SP Pune University	33	Mar. 03
Government College of Engineering, Avasari	75	Mar. 10
Army Institute of Technology, Pune	40	Mar. 19
S. N. D. T. Arts & Commerce College for Women, Pune	44	Mar. 19

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Picture Gallery

Pictures during the workshop on **Scientific Applications on PARAM Yuva II**

Workshop Poster.

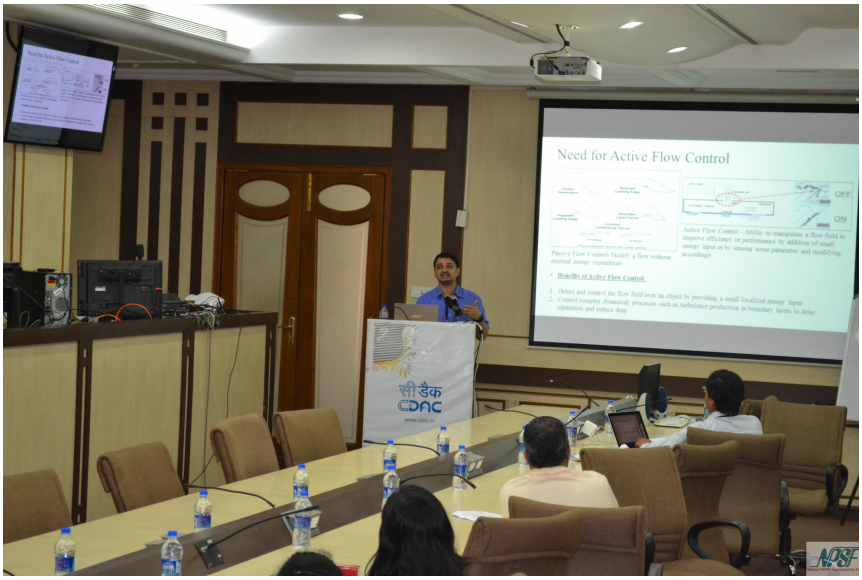
Dr. Themalarchelvi Rathinavelan (IIT, Hyderbad) during the talk.

Dr. Sivasubramanian Gopalakrishnan (IIT, Bombay) during the talk.

Dr. Santosh Ansumali (JNCASR, Bangalore) during the talk.

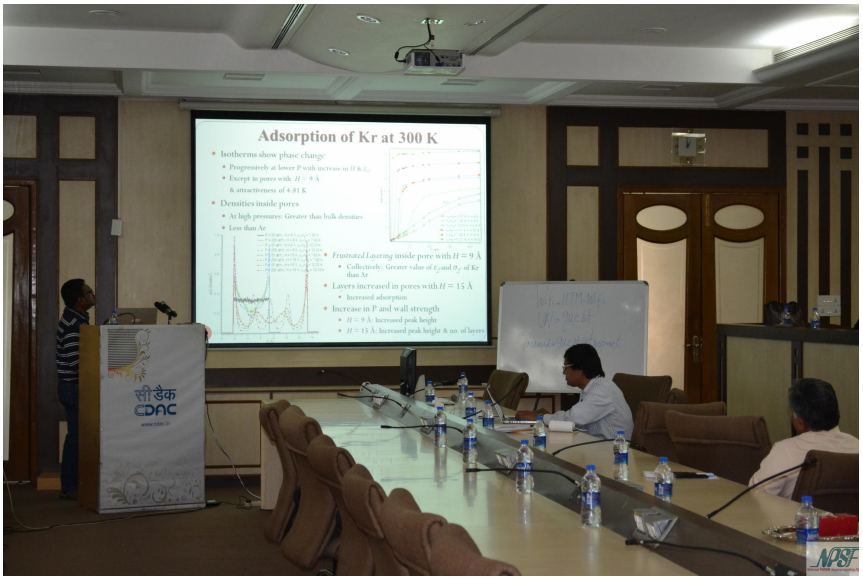
Dr. Prasenjit Ghosh (IISER, Pune) during the talk.

Prof. Murali Damodharan (IIT, Gandhinagar) during the talk.



Mr. Aditya Gupte (IIT, Bombay) during the talk.

Mr. Mandar Kulkarni (IISER, Pune) during the talk.

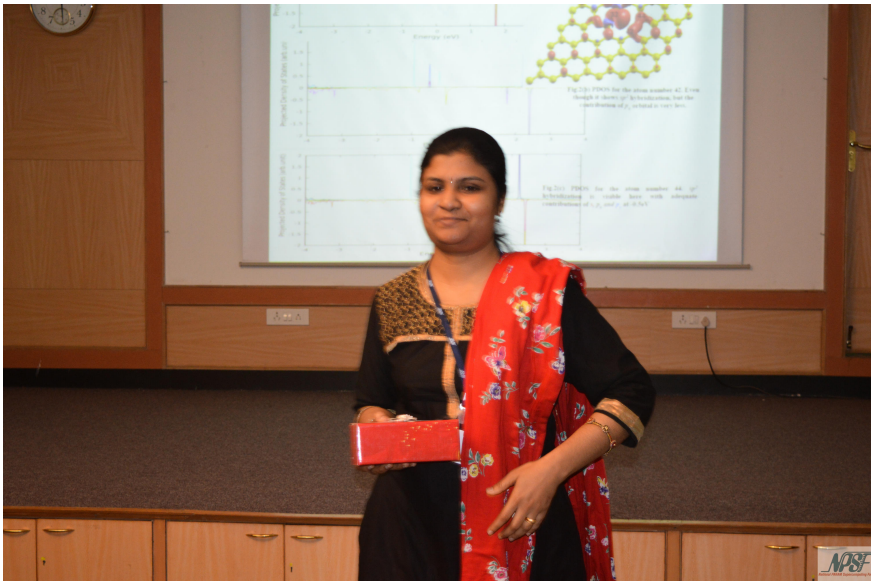


Mr. Angan Sengupata (IIT, Bombay) during the talk.

Dr. Arnab Mukherjee (IISER, Pune) with Prof. Mahendra Verma (IIT, Kanpur).

Dr. Vaishali Shah (S P Pune Univ.) during the talk.

Dr. Mrinalini Deshpande (HPT Arts & RYK Sci. Coll., Nasik) during the talk.



Ms. Priya Francis (S P Pune Univ.) during the talk.

Dr. Amol Rahane (VKF, Gurgaon) with Dr. Uddhavesh Sonavane (C-DAC).

Ms. Nalini Sharma (Himachal Pradesh Univ.) with Dr. Uddhavesh Sonavane (C-DAC).

Dr. Vikas Kashid (S P Pune Univ.) with Prof. Abir De Sarkar (INST, Mohali).

Dr. Manali Joshi (S P Pune Univ.) with Prof. Abir De Sarkar (INST, Mohali).

Dr. Avinash Kale (CBS, Mumbai) during the talk.

Dr. Uddhavesh Sonavane (C-DAC) with Prof. Abir De Sarkar (INST, Mohali).

Session in progress at Varahamihir hall.

PARAM YuvaII at a glance.

C-DAC Science Day Celebrations, Feb. 28, 2015: NPSF stall.

C-DAC Science Day Celebrations, Feb. 28, 2015: NPSF stall (contd.).

C-DAC Science Day Celebrations, Feb. 28, 2015: NPSF team volunteers.

Appendix A

Institutions and Projects

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.

P.T.O

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

Institution	Project	Chief Investigator	No. of users
Ahmednagar College	Investigation of semiconducting nano clusters using first principle calculations	Dr. Pardip Shelke	1
Amity University	DFT based chemical, structural, optical and magnetic study of functionalized Graphene nanoribbons	Dr. Siddheshwar Chopra	1
Anna University	Investigation of electronic structure and related properties of compound semiconductors	Dr. Sankar Sambasivam	2
BARC	Structure and dynamics of deposited metal clusters	Dr. Chiranjib Majumder	1
CBS, Mumbai	Conformational dynamics of actin and its regulators	Dr. Avinash Kale	2
CIFRI, Kolkatha	Bio-prospecting of genes and allele mining for abiotic stress tolerance	Dr. Bijay Kumar Behera	2
CMRCET, Hyderabad	Detecting near duplicates for web crawling	Mr. Varahabatla Narayana	2
Carnegie Mellon University	Adsorption of ionic liquids on graphene surface	Dr. Nilesh R. Dhumal	1
CECRI, Karaikudi	Metal chalcogenides nanostructures for catalytic and electrochemical applications	Dr. P. Murugan	1
Central Univ. of Bihar	Molecular Dynamics study of thermo-stability of archael protein	Dr. Krishna Kumar Ojha	1
Central Univ. of Gujarat	Computational approach to the development of nanostructured catalyst of hydrogen production	Dr. Prakash C. Jha	2
	Computer modelling of skin sensitization potentials and reactivity of chemicals	Dr. Prakash C. Jha	2
Delhi University	MD Simulations project of Delhi University	Prof. Parbati Biswas	2
Govt. College, Tonk	Study of P- and P, T- odd effects in heavy polar diatomics	Dr. Manu Sikarwar	1

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Table A.1 – *Continued from previous page*

Institution	Project	Chief Investigator	No. of Users
Gunanak Dev University	To study the atomic and electronic structure of III-V semiconductor nanostructures	Prof. S. S. Sekhon	1
Himachal Pradesh Univesity	First priciples static, dynamic and electronic properties of liquid metal alloys	Prof. Pradeep K Ahluwalia	3
HPT Arts & RYK Sc. Coll., Nasik	Theoretical study of structural, electronic and magnetic properties of nanomaterials	Dr. Mrinalini Deshpande	2
IAAST, Guwahati	Ab initio calculations of shape memory heusler alloys	Dr. Munima B. Sahariah	3
IIA, Bangalore	Computational many body theory of atoms and molecules	Prof. Bhanu Pratap Das	10
IIIT, Delhi	Explore the benefit of deep neural network for various tasks related to egocentric videos	Dr. Chetan Arora	4
IISc Bangalore	The process of protein folding/aggregation which are responsible for species such as alzheimers	Dr. Govardhan P. Reddy	1
	Defects in Oxides	Dr. Manish Jain	4
	A Robust middleware for job management in supercomputer systems	Prof. Sathish Vadhiyar	1
	Computational Electromagnetics on Intel MIC	Mr. Yoginder Kumar Negi	1
IISER Pune	Mechanistic investigation of photo tautomerization and fluorescence quenching	Dr. Anirban Hazra	4
	Multiscale simulation of shear of miceller systems	Dr. Apratim Chatterji	3
	Coarse Grained Models for Active Matter Simulations	Dr. Apratim Chatterji	2
	Modelling semiflexible polymeric self assembly using a novel 2-body potential	Dr. Apratim Chatterji	2
	Soft Matter in extensional flow using coarse grained simulations	Dr. Apratim Chatterji	2
	Structural deformations of DNA and relation to intercalation mechanism	Dr. Arnab Mukherjee	7

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Table A.1 – *Continued from previous page*

Institution	Project	Chief Investigator	No. of Users
	Molecular modelling and dynamics of polymers, gas hydrates and ionic liquids: An alternative energy initiative	Prof. Arun Venkatanathan	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
	Computing translocation time of polypeptides using milestorming Research	Dr. Srabanti Chaudhury	2
IISER Mohali	Simulating evolution of neutral hydrogen in galaxies in the early universe	Prof. Jasjeet Bagla	1
IISER Thiruvananthapuram	Quantum chemical studies on understanding the interactions of molecules and molecular clusters with graphyne and graphdiyne	Dr. R. S. Swathi	3
IIT Bhubaneswar	Aerodynamic characterization of natural laminar flow	Dr. Yogesh G. Bhumkar	2
IIT Bombay	High Performance Computing initiative	Prof. Amitabh Bhattacharya	150
	Developement of Galerkin Methods	Dr. S. Gopalakrishnan	1
IIT Delhi	Testing of CESM Model	Prof. Krishna M. AchutaRao	3
	Molecular dynamics and trajectory analysis	Dr. Manish Agarwal	1
	System familiarization	Prof. Subodh Kumar	1
IIT Gandhinagar	High fidelity computational engineering	Prof. Murali Damodaran	6
	Using computational approaches MD and QM, to gain insight into hOGT mechanism	Dr. Sairam S Mallajosyula	2
IIT Guwahati	Electronic structure and dynamics	Prof. Aditya N Panda	3
	Electron molecule scattering	Dr. Manabendra Sarma	3
	Atomistic simulation of fast ion transport in solids	Dr. Padma Kumar Padmanabhan	3

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Table A.1 – *Continued from previous page*

Institution	Project	Chief Investigator	No. of Users
	First principles based investigations of shape memory alloys and oxide multiferroics	Prof. Subhradip Ghosh	2
	Electronic structure and magnetic properties of spinel multiferroics	Prof. Subhradip Ghosh	2
	Search for new multifunctional magnetic materials in Heusler structure	Prof. Subhradip Ghosh	2
	Optical properties of perovskite based solar cells	Prof. Subhradip Ghosh	1
	Hydrophobic interactions in different chemical environment	Dr. Sandip Paul	5
IIT Hyderabad	First principles studies on optical, geophysical and superconducting materials	Dr. V. Kanchana	5
	Structure and dynamics of RMA duplexes comprising of trinucleotide repeat expansion	Dr. Thenmalarchelvi Rathinavelan	1
	Structure and dynamics of E.coli outer membrane lectin	Dr. Thenmalarchelvi Rathinavelan	2
IIT Jodhpur	Magnetic functionalization and magnetotransport properties of graphene	Dr. Ambesh Dixit	1
	Theoretical study on lithium ion batteries	Dr. Ambesh Dixit	2
IIT Kanpur	Shape and size effects of nanoparticles on the properties of polymer nanocomposites	Prof. Jayant K. Singh	5
	Magnetohydrodynamics turbulance studies of liquid metals and dynamo	Prof. Mahendra K. Verma	7
	Thunder storm simulation	Prof. Sachidanand Tripathi	1
	Study of complex fluid flows past bluff bodies	Prof. Sanjay Mittal	1
	Study of flow instability, transition and turbulence using high accuracy methods	Prof. Tapan K. Sengupta	3
IIT Kharagpur	To find the interfacial strength in CNT amine epoxy composite	Prof. Baidurya Bhattacharya	4

Continued on next page

Table A.1 – *Continued from previous page*

Institution	Project	Chief Investigator	No. of Users
	To study the impact of land use changes on changing climate over Indian region	Dr. Manabottam Mandal	1
	Intra-seasonal and inter-annual variability studies along the Indian Coasts	Dr. C. Shaji	1
	Aerosol modelling	Prof. Shubha Verma	1
IIT Patna	Immersed boundary method based fluid structure interaction	Dr. Somnath Roy	4
IIT Ropar	H_2 storage and fuel cell materials for renewable energy	Dr. T. J. Dhilip Kumar	3
	Hyper velocity projectile impact	Dr. Navin Kumar	3
	Electronic band Structure calculations of GNRs	Dr. Rakesh Kumar	2
INST, Mohali	Atomic scale design of novel nanomaterials for clean energy and devices	Prof. Abir De Sarkar	5
ISRO			
National Remote Sensing Centre	National carbon project	Dr. M. M. Ali	2
Sathish Dhawan Space Center	Weather Research and Forecasting Model Runs	Dr. M. Rajasekhar	1
Space Applications Centre	Real Time Short Range Weather Forecasting	Dr. P. K. Pal	1
Vikram Sarabhai Space Centre	Aerosol radiative forcing over India	Dr. S. Suresh Babu	1
IUCAA, Pune	Magnetic fields of accreting neutron stars	Prof. Sukanta Bose	2
	Prototyping LIGO data analysis software on HPC Cluster	Prof. Sukanta Bose	3
Jiwaji University	Analysis of electronic and mechanical properties of some heusler alloys and ternary alloys	Dr. Dinesh C. Gupta	3
JMI, Delhi	Variational Monte Carlo study of light nuclei	Prof. Qamar Nasir Usmani	1
JNCASR, Bangalore	Fluid dynamics of clouds	Prof. Roddam Narasimha	4
	Development of a simple and accurate fast 3D numerical method capable of handling moving boundaries	Dr. Santosh Ansumali	2

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Table A.1 – *Continued from previous page*

Institution	Project	Chief Investigator	No. of Users
	Density Functional theory studies of nanosystems	Prof. Shobhana Narasimhan	2
JNU	Entrophy and free energy calculation	Prof. Indira Ghosh	2
MIT, Pune	Simulation and analysis of flow inside a scramjet	Mr. Girish Barpande	1
Manipal University	Porting and tuning of CFSv2.1.8 on PARAM Yuva II	Ms. Jimcymol James	2
NABI, Mohali	Study assembly and annotation of genome and trascriptoms to idetify SNP makrkers from public domains and through international and national collaborations	Mr. Shrikant Mantri	1
NCL, Pune	Investigation of finite temperature behaviour of finite size systems	Dr. Kavitha Joshi	4
	Study of effects of point mutations on the conformational dynamics	Dr. Neelanjana Sengupta	1
	Computational structure-function correlation in biomolecular Systems	Dr. Suman Chakrabarty	1
NCRA, Pune	Search for pulsars and transients	Dr. Jayanta Roy	1
	Software backend for the Ooty radio telescope	Dr. Jayaram N Chengalur	1
	Pulsar data analysis	Mr. Venkata Subramani	3
	Development on MIC based software correlator	Dr. Vishweshwar Ram Marthi	1
NIT Calicut	Study of adsorption of organic molecules on oriented metallic surfaces and its applications to development of more effective catalysts	Prof. Raghu Chatanathodi	1
NIT Rourkela	Effects of swirl and rotation on turbulent pipe flow	Dr. Bikash Sahoo	1
PRL, Ahmedabad	Atomic study	Dr. Bijaya Sahoo	3
RRI, Bangalore	Simulating evolution of neutral hydrogen in galaxies in the early universe	Prof. C R Subrahmanya	1
	Testing Xeon Phi Coprocessor	Prof. Sumati Surya	2
RTM Nagpur University	Statistical physics of time delayed system	Prof. Prashant Gade	2

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Table A.1 – *Continued from previous page*

Institution	Project	Chief Investigator	No. of Users
SP Pune University	Computational studies of the aggregation of patchy particles under non-equilibirum conditions	Dr. Ahmed Sayeed	3
	First-principles investigation of semiconductor nanostructures	Prof. Anjali Kshilsagar	2
	Electronic structure calculations	Dr. Bhalchandra S. Pujari	1
	Investigation of physics of confined systems	Prof. Dilip. G. Kanhere	1
	The study of diffusion coefficient of Te on Cd-Te surface(111)	Mr. Ebadollah Naderi	1
	MD simulation of DNMT1	Dr. Manali Joshi	1
	Water cluster and molecule interactions in electric field	Prof. Rajeev Pathak	2
	Molecular Tailoring Approach: Ab initio treatment of large molecules and molecular clusters	Prof. Shridhar R. Gadre	2
	Probing noncovalent interactions using density functional theory	Prof. Shridhar P Gejji	3
	Electronic structure calculations of semiconductors	Prof. S. V. Ghaisas	2
	Investigation of structural and optical properties of semiconducting materials in various forms	Prof. S. V. Ghaisas	1
	Ab initio investigations on nano-biomaterials and ternary alloys	Dr. Vaishali Shah	5
SRM University	Theoretical modeling of novel nanoelectronic devices	Dr. Arjit Sen	3
St. Xavier's College, Ahmedabad	Quantum transport in elemental doped boron nitride monolayer	Dr. Sanjeev Kumar Gupta	1
VKF, Gurgaon	Ab initio studies of materials: nanostructures, defects, surfaces and bulk metallic glasses	Prof. Vijay Kumar	6
VNIT Nagpur	Project on generation of largest prime no.s	Mr. S. Ukesh Kumar	1

Appendix B

Dedicated Slot Booking Facility: Pre-April 2014

This appendix is a summary of dedicated slots (both PARAM Yuva I & Yuva II) from January 2012 till March 2014.

P.T.O

Table B.1: Summary of the utililiztion of dedicated slots: Pre- April 2014

User	Chief Investigator	Institution	Domain	Start Time	Duration	# Nodes
2014						
Dr. Manali Joshi	Dr. Manali Joshi	UniPune	Bio Sc.	2014-02-11 17:00:00:0	*10:0:0:00	64
Dr. Prasenjit Ghosh	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2014-01-16 17:00:00:0	*7:0:0:00	64
2013						
Prof. Shridhar Gadre	Prof. Shridhar Gadre	IIT Kanpur	Chemical Sc.	2013-10-08 18:30:00:0	67:0:0:0	4
Dr. Bheema Lingam C	Prof. Vijay Kumar	VKF Gurgoan	Material Sc.	2013-09-18 10:01:00.0	14:0:0:00	32
Mr. Sahidul Islam	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2013-09-02 10:01:00.0	14:23:0:00	30
Mr. Souvik Pal	Prof. Subhradip Ghosh	IIT Guwahati	Material Sc.	2013-08-01 23:22:00.0	10:0:0:00	32
Ms. Ancymol Thomas	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2013-08-01 09:30:00.0	14:23:59:00	48
Mr. Sudipta Banerjee	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2013-07-17 09:30:00.0	14:23:59:00	40
Prof. Subhradip Ghosh	Prof. Subhradip Ghosh	IIT Guwahati	Material Sc.	2013-07-13 23:27:00.0	10:10:30:00	32
Dr. Kavita Joshi	Dr. Kavita Joshi	NCL Pune	Chemical Sc.	2013-07-01 10:01:00.0	14:23:59:00	48
Dr. Satyaban Bishoyi R	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2013-06-28 09:30:00.0	14:23:59:00	40
Ms. Deepika Goyal	Dr. Rakesh Kumar	IIT Ropar	Material Sc.	2013-06-24 14:05:00:0	03:19:55:00	64
Mr. Sahidul Islam	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2013-06-24 10:01:00.0	10:1:1:00	32
Mr. Hungyo Kharerin	Prof. A. Bhattacharya	IIT Bombay	Bio Sc.	2013-06-22 1:01:00:0	7:0:0:00	30
Mr. A. Ranganathan	Prof. A. Bhattacharya	IIT Bombay	Chemical Sc.	2013-06-14 01:01:00:0	6:0:0:00	40
Dr. Bheema Lingam C	Prof. Vijay Kumar	VKF Gurgoan	Material Sc.	2013-06-13 10:01:00.0	14:0:0:00	30
Mr. Basanta Samala	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2013-06-13 09:30:00.0	14:23:59:00	40
Ms. Prajakta Sapre	Prof. A. Bhattacharya	IIT Bombay	Comput. Sc.	2013-06-13 09:01:00.0	2:10:0:00	20
Prof. Mahendra Verma	Prof. Mahendra Verma	IIT Kanpur	CFD	2013-06-07 14:00:00:0	†49:0:0:0	64
Ms. Deepika Goyal	Dr. Rakesh Kumar	IIT Ropar	Material Sc.	2013-06-13 14:00:00:0	†15:0:0:0	64
Ms. Deepika Goyal	Dr. Rakesh Kumar	IIT Ropar	Material Sc.	2013-07-13 14:00:00:0	†18:0:0:0	64
Dr. Kavita Joshi	Dr. Kavita Joshi	NCL Pune	Chemical Sc.	2013-08-13 16:00:00:0	‡6:0:0:0	64
Prof. Mahendra Verma	Prof. Mahendra Verma	IIT Kanpur	CFD	2013-09-08 14:00:00:0	†24:0:0:0	64

Continued on next page

Table B.1 – *Continued from previous page*

User	Chief Investigator	Institution	Domain	Start Time	Duration	# Nodes
2012						
Mr. Arya Dhar	Prof. B. P. Das	IIA Bangalore	Atm./Mol. Sc.	2012-12-30 10:25:0:0	30:0:0:0	2
Mr. Kuldeep Sharma	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2012-11-01 11:01:00.0	14:23:59:00	120
Mr. Sahidul Islam	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2012-10-15 23:59:00.0	14:23:59:00	28
Dr. Kavita Joshi	Dr. Kavita Joshi	NCL Pune	Chemical Sc.	2012-10-15 11:01:00.0	14:23:59:00	100
Mr. Abhishek Shrivastav	Ms. Richa Rastogi	C-DAC	Geo Sc.	2012-10-03 11:01:00.0	12:0:0:00	64
Prof. Arun Venkatanathan	Prof. Arun Venkatnathan	IISER Pune	Chemical Sc.	2012-09-27 01:01:00.0	14:23:59:00	25
Dr. Manabottam Mandal	Dr. Manabottam Mandal	IIT Kharagpur	Climate Sc.	2012-09-13 10:01:00.0	14:23:59:00	36
Mr. Abhishek Shrivastav	Ms. Richa Rastogi	C-DAC	Geo Sc.	2012-07-31 11:01:00.0	14:23:59:00	60
Mr. Abhishek Shrivastav	Ms. Richa Rastogi	C-DAC	Geo Sc.	2012-07-02 11:01:00.0	14:23:59:00	40
Prof. Vijay Kumar	Prof. Vijay Kumar	VKF Gurgoan	Material Sc.	2012-06-30 11:01:00.0	14:23:59:00	60
Dr. Manabottam Mandal	Dr. Manabottam Mandal	IIT Kharagpur	Climate Sc.	2012-06-30 10:01:00.0	14:0:0:00	25
Mr. Sudipta Banerjee	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2012-06-15 13:01::00:0	14:0:0:0	64
Prof. Shridhar Gadre	Prof. Shridhar Gadre	IIT Kanpur	Chemical Sc.	2012-05-31 12:01:00.0	14:23:59:00	64
Mr. Swagata Bhaumik	Prof. Tapan Sengupta	IIT Kanpur	CFD	2012-05-15 10:01:00.0	14:23:59:00	128
Ms. Ancymol Thomas	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2012-04-30 17:45::00:0	15:0:0:0	1
Prof. Vijay Kumar	Prof. Vijay Kumar	VKF Gurgoan	Material Sc.	2012-04-30 11:01:00.0	10:0:0:00	20
Dr. Satyaban Bishoyi R	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2012-04-27 12:01:00.0	14:0:0:00	64
Dr. Kavita Joshi	Dr. Kavita Joshi	NCL Pune	Chemical Sc.	2012-04-12 11:01:00.0	14:23:59:00	64
Ms. Ancymol Thomas	Ms. Akshara Kaginalkar	C-DAC	Climate Sc.	2012-03-23 11:01:00.0	14:23:0:00	32
Prof. Shridhar Gadre	Prof. Shridhar Gadre	IIT Kanpur	Chemical Sc.	2012-03-22 12:01:00.0	14:0:0:00	32
Dr. Kavita Joshi	Dr. Kavita Joshi	NCL Pune	Chemical Sc.	2012-12-08 02:00:00:0	§7:0:0:0	64

*These slots are in chunks (of 16 hrs 55 min duration) available for consecutive days.
†These slots are in chunks (of 20 hrs duration) available for consecutive days.
‡These slots are in chunks (of 18 hrs duration) available for consecutive days.
§These slots are in chunks (of 7 hrs duration) available for consecutive days.

Appendix C

Ph.D Theses by NPSF users

The following are the Ph.D theses by NPSF users (PARAM Yuva I & Yuva II) prior to 2014-15 that acknowledge the use of computing time on NPSF resources.

1. **Ab initio electronic structure calculations of semiconductor quantum dots** (August, 2012)
   Student: Mr. Sachin P. Nanvati, Dept. of Physics, University of Pune
   Supervisor: Prof. S. V. Ghaisas (Dept. of Electronic Science)

2. **A study of the atomic and electronic structure of III-V compound semiconductor nanostructures** (March, 2013)
   Student: Ms. Prabhsharan Kaur, Dept. of Physics, Guru Nanak Dev University, Amritsar
   Supervisor: Prof. S. S. Sekhon

3. **Algorithm Development for Building and Analysis of Molecular clusters : A quantum Chemical Study** (April, 2013)
   Student: Mr. Sachin D. Yeole, Dept. of Chemistry, University of Pune
   Supervisor: Prof. Shridhar R. Gadre

4. **Theoretical study of structural, magnetic and optical properties of metal oxide nanostructures** (May, 2013)
   Student: Mr. Amol B. Rahane, Dept. of Physics, H. P. T. Arts & R. Y. K. Science College, Nasik & University of Pune
   Supervisors: Dr. Mrinalini Deshpande & Prof. D. G. Kanhere

5. **Numerical simulation of inhomogeneous transitional and turbulent flows** (July, 2013)
   Student: Mr. Swagata Bhaumik, Dept. of Aerospace Engineering, IIT, Kanpur
   Supervisor: Prof. Tapan Sengupta

6. **Structure, electronic and magnetic properties of Au, Ni nanowires and their alloys** (November, 2013)
   Student: Mr. Vikas T. Kashid, Dept. of Physics, University of Pune
   Supervisors: Dr. Vaishali Shah (ISSC, UniPune) & Dr. H. G. Salunke (BARC)

7. **Coarse-grained molecular simulations of polymers and nanocomposites: Structure, dynamics and phase behavior** (February, 2014)
   Student: Mr. Tarak K. Patra, Dept. of Chemical Engineering, IIT, Kanpur
   Supervisor: Prof. Jayant K. Singh

Appendix D

Workshops organized/participated: Pre-April 2014

The workshops conducted by NPSF prior to April 2014 are listed below:

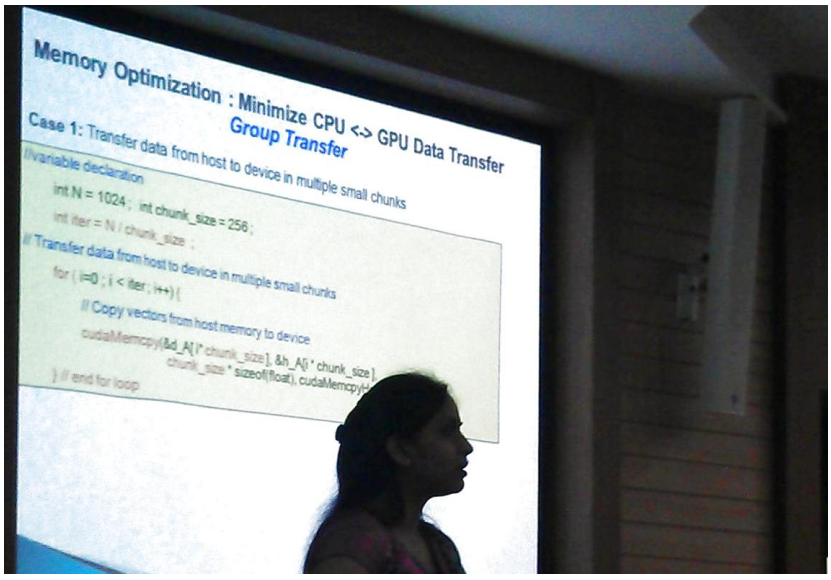
- Conducted workshop on **Application Performance Optimization on HPC Clusters** on Oct. 26, 2012 at IIT, Bombay. About *fifty* participants attended the workshop. The topics covered were:

  i. CUDA and OpenCL Optimizations - Part I by Ms. Chaitali Chandratre, Ms. Nisha Agrawal & Mr. Samrit Maity

  ii. CUDA and OpenCL Optimizations - Part II by Mr. Samrit Maity & Ms. Nisha Agrawal

  iii. Processor/node architectures : Tigerton, Nehalem and Sandy Bridge by Mr. Maneesh Kumar

  iv. Application profiling and analysis using tools eg. HPC ToolKit by Mr. Rishi Pathak



Ms. Nisha Agrawal during the workshop at IIT, Bombay.

Participants of the workshop at IIT, Bombay.

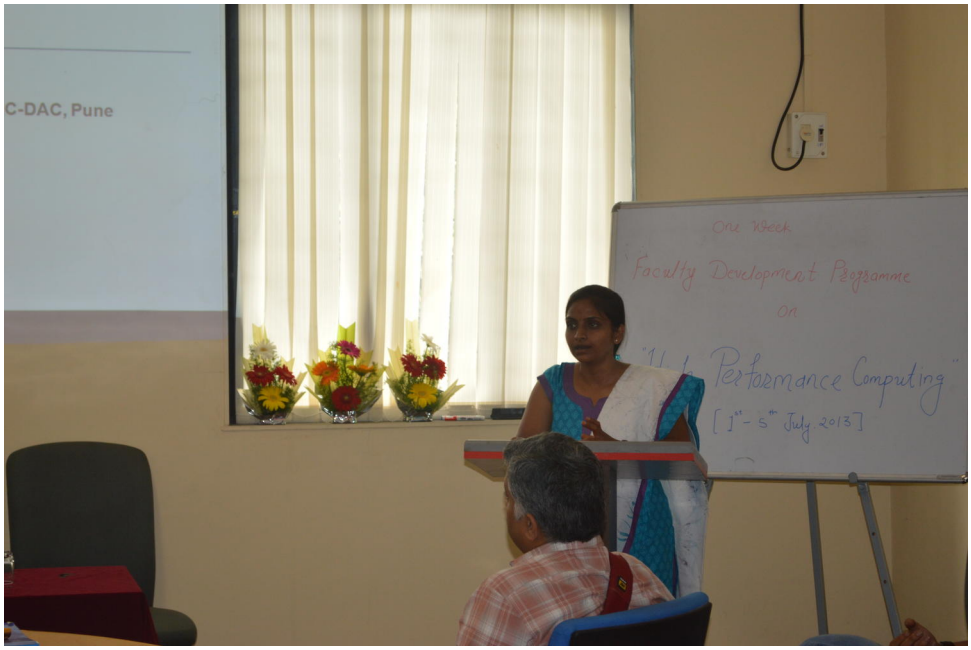
- Conducted workshop on **National Supercomputing Mission** on Feb. 8, 2013 at VITS Hotel, Pune.

  This workshop was coordinated by the then Honourable Secretary, DeitY, GoI, Shri J . Satyanarayana in the presence of Prof. N. Balakrishnan of IISc, Bangalore, Dr. Vijay Bhatkar, founder Executive Director of C-DAC and members of C-DAC senior managment, Prof. Rajat Moona, Director General, Dr. Hemant Darbari, Executive Director, C-DAC, Pune, Dr. Sarat Chandra Babu, Executive Director, C-DAC, Bangalore and Dr. Pradeep K. Sinha, Senior Director, HPC. Over *sixty* delegates representing Institutes, National Labs, NITs, IITs, and Universities, *participated in the brainstorming session to discuss the future of HPC in India.* There were presentations from several stakeholders across different ministries covering different domain of applications. Several members (over *fifty*) of C-DAC HPC groups also participated in the workshop. This workshop coincided with the release of PARAM Yuva II to the Indian scientific community.

- Conducted *a day long session* on Jul. 1, 2013 during the **Faculty development program** (FDP) on *High Performance Computing* during Jul. 1-5, 2013 at Walchand College of Engineering (WCE), Sangli under Technical Education Quality Improvement Programme (TEQIP). There were around *sixty* The following topics were covered in the workshop:

  i. Unconventional Computing by Dr. Sandeep K. Joshi
  ii. Scientific applications on HPC Systems - Performance and Scaling challenges by Dr. V. Venkatesh Shenoi
  iii. Profiling and performance analysis tools - Intel Vtune by Ms. Chaitali Chandratre
  iv. Performance tuning of applications using HPC Toolkit by Ms. Nisha Agrawal
  v. Technologies for Petascale and Exascale HPC by Mr. Rishi Pathak
  vi. A review of power & energy consumption optimization in HPC by Mr. Rishi Pathak

Dr. Sandeep Joshi (top) and Ms. Chaitali Chandratre (bottom) during the FDP at WCE .



Ms. Nisha Agrawal (top) and Mr. Rishi Pathak (bottom) during the FDP at WCE.

PARAM Series of Supercomputers

PARAM Yuva II

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