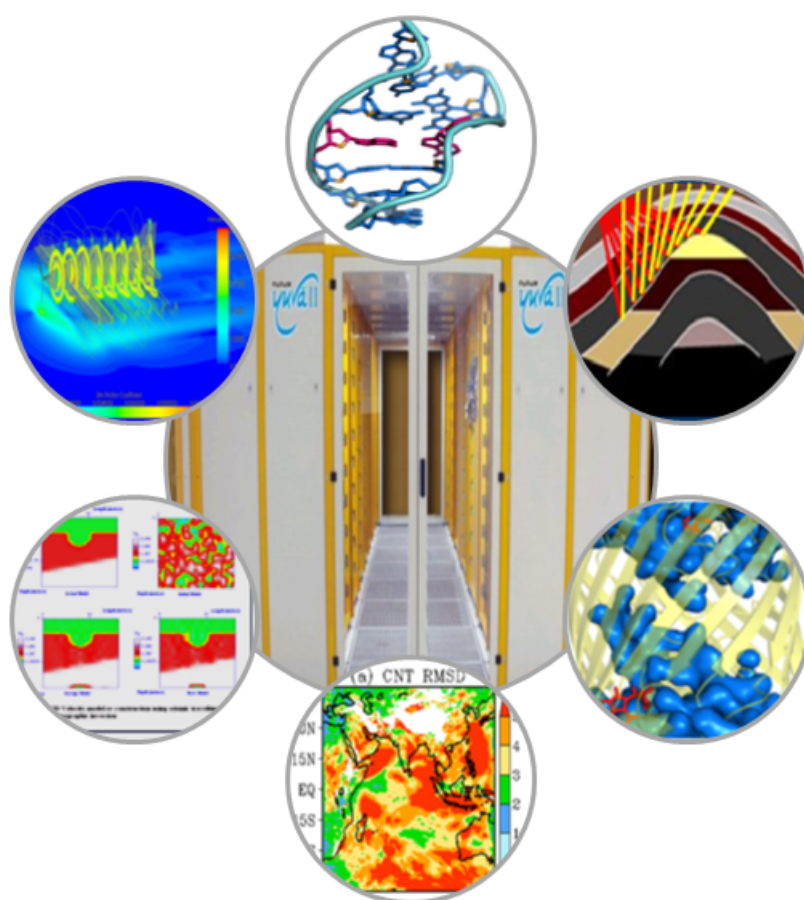


National PARAM Supercomputing Facility

ANNUAL REPORT FY 2015-16



Greetings from Director General



I feel extremely pleased and proud to place this exclusive report of the activities at National PARAM Supercomputing Facility (NPSF) for the financial year 2015-16.

PARAM Yuva-II system, the first hybrid supercomputer in PARAM series at NPSF, C-DAC, Pune, continued to offer its services to the scientific and academic community in the third year of its operation. NPSF reached new heights with an all time high count of the total number of publications in the peer-reviewed National/International journals and Ph.D. thesis submitted by users of the NPSF, to name a few.

I congratulate all members of NPSF team for their tireless and unending contribution in providing support to over 800 users from 72 R&D and academic institutions who are using PARAM Yuva II system for their research work. The requirement of same is expected to grow manifold in the coming years with the advent of National Supercomputing Mission (NSM) which has been approved by Govt. of India.

NPSF with its earned expertise of over more than two decades has a big and challenging role to play in the coming years ahead. I extend my best wishes and whole hearted support to NPSF and its members for all their future endeavors.

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

Prof. Rajat Moona
Director General, C-DAC

Greetings from Executive Director



At the foremost, my sincerest congratulations to all the scientists and researchers from all across the country, who have been and are using our NPSF resources for their research needs. It is indeed gratifying to note how this community has grown over the years to reach a sizeable population. With our rich experience in HPC, the future indeed looks bright for C-DAC as we poise ourselves for the next generation leap into petascale and exascale supercomputing systems. At the same time, I am also proud to note that C-DAC is the only organization in the nation offering HPC resources to both academic and research organizations. The milestones we have crossed and the accolades that we continue to receive are partly due to our perseverance, along

with the support and faith of our parent body, the Department of Electronics and Information Technology (DeitY), Government of India. It is their unwavering confidence in C-DAC's capabilities that has brought us to the position of frontrunner for the highly prestigious National Supercomputing Mission (NSM) initiated by the Government of India.

I am extremely hopeful that C-DAC will continue to enhance its strengths, building its capabilities through experience and collaborations to work on newer and challenging areas that will make a difference to the nation and its citizens.

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

Greetings from Head of Department

This report is a testament to the immense commitment and effort our team has put in operating the NPSF. As in the previous years, our team has ensured that the users computing requirements are met as completely and transparently as possible. During the past year, the NPSF user community has crossed 800+ users and the total number of jobs executed has risen to 1,92,708. The number of research thesis and publications by our users is a clear testament to our efforts to provide the highest usability and availability levels.

While operating and maintaining a large facility like NPSF is a challenge in terms of system reliability and availability, there was also a good deal of preparatory work that was carried out in the background to build and provide new services to the HPC community. I am sure that our users will benefit greatly by this. A good deal of effort was also devoted to the National Supercomputing Mission (NSM) that was approved this year, and the NPSF team is excited at the challenges that lie ahead.

We thank our Director General, Executive Director and more importantly, our valuable users for supporting us in our efforts to provide the best possible supercomputing platform.

HAPPY COMPUTING!

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

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1

Thriving the HPC

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 69th in the Top500 list released in November 2008 at the Supercomputing Conference in Austin, Texas, United States.

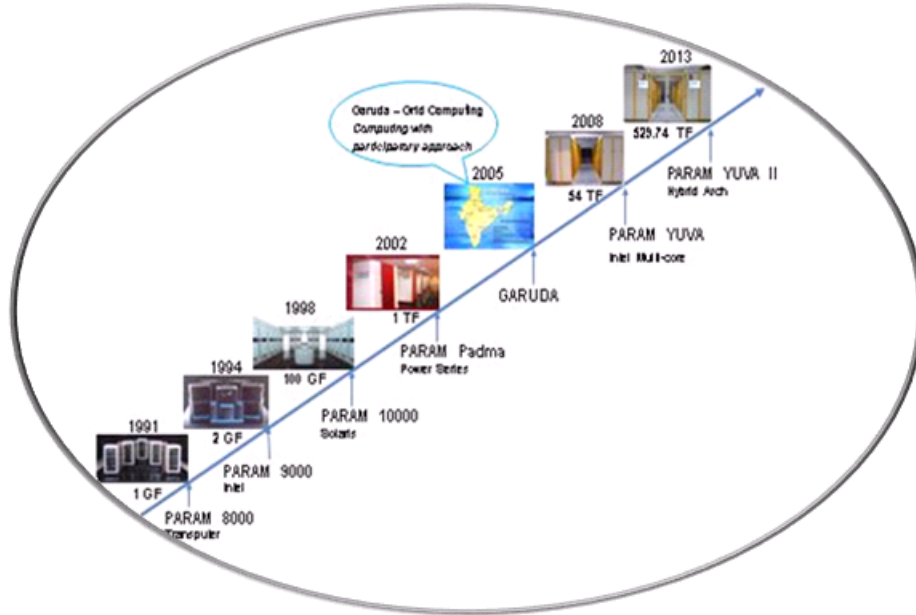


Figure 1.1: HPC evolution @ C-DAC

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/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 FY 2015-16.

PARAM Yuva: Operational Year 2008-2012, Peak Perf. 54 TFlop/s, Highest Rank in Top500 69

PARAM Yuva II:Operational from Year2013, Peak Perf. 529.4 TFlop/s,Highest Rank in Top500 69

2

PARAM Yuva II by Numbers

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

1,92,708 Jobs completed processing.

251 Rank as per November, 2015 Top500 list.
[Highest Rank achieved in Top500 supercomputer across globe :
69 in June, 2013 Top500 <http://www.top500.org>]

96 Rank as per November, 2015 Green500 list.
[Highest Rank achieved in Green500 supercomputer across globe :
44 in November, 2013 Green500 <http://www.green500.org>]

812 Users.

72 Institutions.

221 Projects.

21 Completed Ph.D's.

118 Publications.

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

3

Year 2015 - 2016 in Review

2015

May

Maintenance activity of PARAM Yuva II undertaken from May 5th to 7th, 2015 (1 day 23 hours). Major activities performed during maintenance are Intel Manycore Platform Software Stack (Intel MPSS) upgradation, installation of Intel(R) Parallel Studio XE 2015, network configuration and scheduler policy changes.

June

HPC workshop on "Performance optimization and parallelization techniques" was organized by NPSF on June 15, 2015 at C-DAC Pune. 20+ C-DAC members participated in the workshop and got exposure to various optimization techniques.

July

HPC workshop on "Hands-on sessions on performance optimization techniques, performance analyzing and profiling tools" was organized by NPSF on July 03, 2015 at C-DAC, Pune. 20+ C-DAC members participated in the workshop and got hands-on experience of various optimization techniques and performance analyzing and profiling tools.

HPC workshop on "Parallel Computing, performance optimization techniques, performance analyzing and profiling tools" was organized by NPSF along with IISER Mohali, on July 14-15, 2015 at IISER Mohali. More than 35 participants from research institutions/organizations like IISER, INST, NABI, DRDO participated in the workshop and got exposure and hands-on experience on parallel computing, performance optimization techniques, performance analyzing and profiling tools.

August

On August 13, 2015, Mr. Pankaj Dorliker delivered invited talk on "Computer Architecture for Scientific Computing" to the students of Savitribai Phule Pune University. The speaker of the talk was invited by Dr. Vaishali Shah, Assist.Prof, CMS Dept., S. P. Pune University.

September	On September 11, 2015, Mr. Y. S. Swarup delivered invited talk on "HPC Cooling Technologies" at ACR TrendZ 2015 in Pune, organized by ISHRAE.
December	<p>On December 16, 2015, Mr. Y. S. Swarup delivered invited talk on "HPC Technologies" at Govt. college of Engg, Karad, as a part of Faculty Development Program.</p> <p>Introduced Dedicated Slot Booking for slots in chunks of 14 hrs 55 minutes duration, on December 22 for the period from January 11 to March 07, 2016.</p>
2016	
January	<p>On January 22, 2016, Mr. Y. S. Swarup delivered invited talk on "HPC Technologies & Job opportunities" to the students of SKBR College, Am-lapuram (Andhra Pradesh). Students got exposure of HPC Technologies.</p> <p>Visit to Institute of Physics (IOP), Bhubaneswar, by Dr. Sandeep Joshi & Dr. Venkatesh Shenoi during January-February 2016, as part of PARAM Yuva II promotional activities.</p>
February	<p>On February 13, 2016, Ms. Nisha Agrawal delivered invited talk on "Introduction to OpenCL Computing" for faculties from various engineering institutes of Maharashtra at Pune Institute of Computer Technology (PICT), Pune. The talk was delivered as a part of faculty development program, upon invitation from PICT, Pune.</p> <p>As a part of National Science Day celebration at C-DAC on February 28, 2016, NPSF team participated in the event and showcased the activities related to PARAM Yuva II. Around 1496 visitors (Students from various colleges and schools) from Pune and nearby districts like Ahmednagar, Satara, Sangli and Kolhapur enjoyed the technical sessions and walk-through of PARAM Yuva-II.</p>
March	Provided PARAM Yuva II computing resources support for International High Performance Computing (IHPC) competition as part of Techkriti 16 organized by IIT, Kanpur between March 7-11 2016.

As we step into the early phase of the implementation of the National Supercomputing Mission (NSM), the inputs from the user community across various domains in terms of the requirements of the computational resources, the storage capacity, I/O behavior of their applications etc. have been collected. Valuable inputs recieved from users, would help us in planning the future systems as well as formulating the usage policies.

4

Computing Resources



Four subclusters

Subcluster 1

220 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, DSBFp

Subcluster 2	<p>Over 100+ nodes cluster of HP Proliant DL580 G5 with</p> <p>Quad socket Intel Xeon X7350 Processor per node</p> <p>Four CPU cores per socket, 2.93 GHz</p> <p>System interconnects: PARAMNet3, Infiniband DDR</p> <p>Partition: DDRp</p>
Subcluster 3	<p>Four nodes cluster of Supermicro SuperServer 1027GR-TRF with</p> <p>Dual socket Intel Xeon E5 2650 (Sandy Bridge) Processor per node</p> <p>Eight CPU cores per socket, 2.6 GHz</p> <p>Two NVIDIA GPU Tesla M2090 per node</p> <p>Infiniband FDR interconnect</p> <p>Partition: GPUp</p>
Subcluster 4	<p>Supermicro 4U AMD SR5690 SMP server with 64 cores</p> <p>Quad socket AMD Opteron 6276 Processor</p> <p>Sixteen CPU cores per socket, 2.3 GHz</p> <p>512 GBytes of RAM</p> <p>Partition: (grouped with) GPUp</p>
Storage	<p>HPC Scratch area with 10 GB/s write bandwidth over Parallel File System</p> <p>Reliable User Home Area: 100TB</p> <p>Backup: 400TB (native capacity)</p>
Software	<p>Operating System: CentOS v6.2, Kernel v2.6.32-220</p> <p>Intel Cluster Studio XE 2013</p> <p>PGI Cluster Development Kit</p>
Applications	<p>Libraries and software for file formats, data bases and math</p> <p>Many scientific applications for material science/quantum chemistry, molecular modelling, fluid dynamics, climate modelling and circuit simulations and many more like aerospace engineering.</p>

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

Partitions and Queues:

The 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
DSBFp	DSBFq †	15 Days	Xeon Phi
SDSp§	SDSq †	14 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 other users for reservation through Dedicated Slot Booking Facility (DSBF).

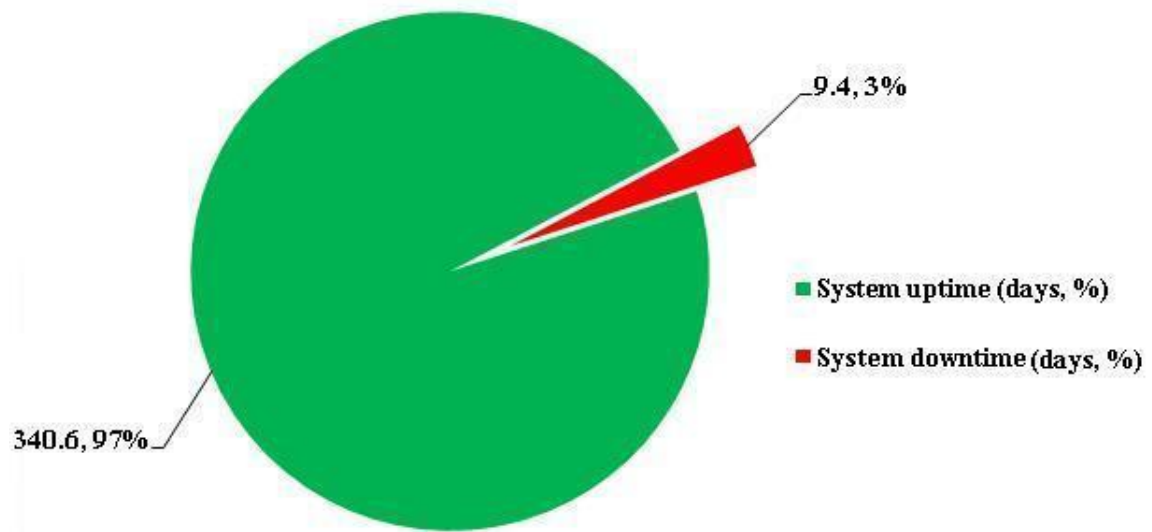
*Queue for jobs with GPU nodes/SMP node.

†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.

PARAM Yuva II availability: (Period: Apr. 1, 2015 - Mar. 31, 2016) [350 Days]



- Uptime: 341 Days
- Maintenance Period: 9 Days
 - May 05, 2015, 11:37 AM May 07, 2015, 11:00 AM [1 Day, 23 Hrs]
 - July 08, 2015, 11:30 AM July 15, 2015, 09:00 PM [7 Days, 9 Hrs]
- System uptime: 97%

Total compute nodes 290(221 nodes of PARAM Yuva II + some preserved old nodes)
Intel Xeon Phi 5110P with 60 cores
More than 49 open source scientific applications/libraries/tools made available
77% of total downtime was due to the cluster ecosystem(power subsystem) failure

5

Growth in HPC User Community

Projects & Users (as of 31 March 2016)

- Number of projects : 221
- Number of users: 812 (across 72 Institutions)
- Number of PhD students: 141

Users across Institutions

Table 5.1: Users across Academic Institutions

Academic Institutions	No. of Users
Ahmednagar College	1
Amity University	1
Aligarh Muslim University	5
Anna University	2
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
Delhi University	2
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	51
IISER, Mohali	1
IISER, Thiruvananthapuram	3

Continued on next page

Table 5.1 – *Continued from previous page*

Academic Institutions	No. of Users
IIT Bombay	178
IIT Bhubaneswar	2
IIT Delhi	8
IIT Guwahati	23
IIT Gandhinagar	10
IIT Hyderabad	16
IIT Jodhpur	8
IIT Kanpur	23
IIT Kharagpur	7
IIT Patna	5
IIT Ropar	8
INST, Mohali	8
JMI University	1
Jiwaji University	3
JNU	2
Manipal University	2
MIT Pune	1
NIT Calicut	1
NIT Rourkela	1
Panjab University	2
PJTSAU, Hyderabad	1
University of Rajasthan	1
RTM Nagpur University	2
SASTRA University, Thanjavur	3
PDU Shekhawati Univ., Sikar	1
SRM University	3
St. Xavier's College, Ahmedabad	1
SP Pune University	32
VNIT Nagpur	1
Total	466

Table 5.2: Users across research institutions

Research Institutions	No. of Users
BARC, Mumbai	1
CBS, Mumbai	2
CIFRI, Kolkata	2
C-DAC	123
CECRI, Karaikudi	4
E-teacher	2
GARUDA	157
IASST, Guwahati	4
ISRO	5
IUCAA, Pune	7
JNCASR, Bangalore	10

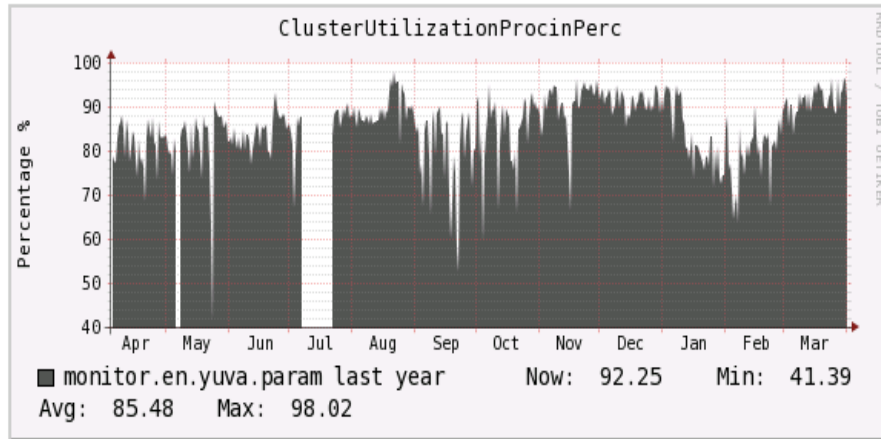
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Table 5.2 – Continued from previous page

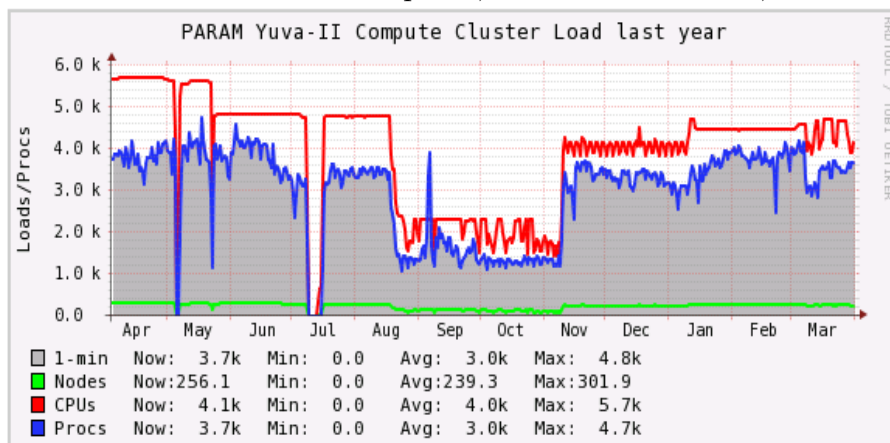
Research Institutions	No. of Users
NABI, Mohali	1
NCL, Pune	6
NCRA, Pune	6
NIC	2
PRL, Ahmedabad	3
RRI, Bangalore	3
SINP, Kolkata	2
Vijay Kumar Foundation, Gurgaon	6
Total	346

PARAM Yuva II System utilization:

Cluster Utilization : April 1, 2015 - March 31, 2016



Cluster load : April 1, 2015 - 31 March 31, 2016



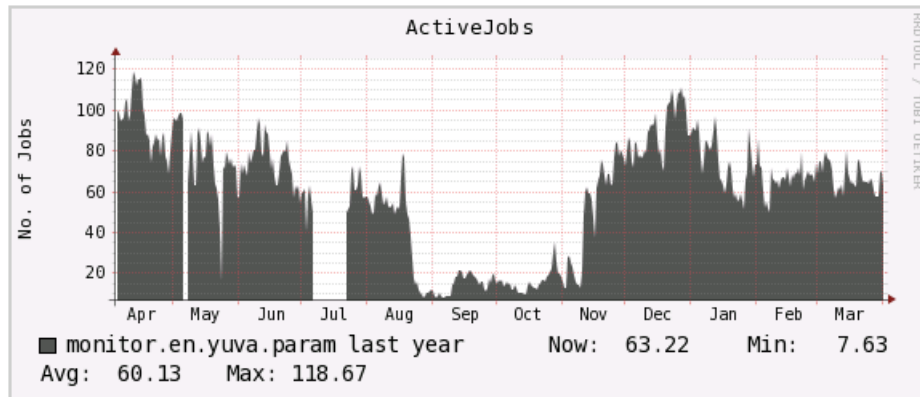
The maintenance activity of PARAM Yuva II accounts for the gaps in the months of May (1 day 23 hours) and July (7 days 9 hours from July 08) in the utilization graph (top).

There was a partial shutdown of PARAM Yuva II (some of the nodes) during the August to November 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:

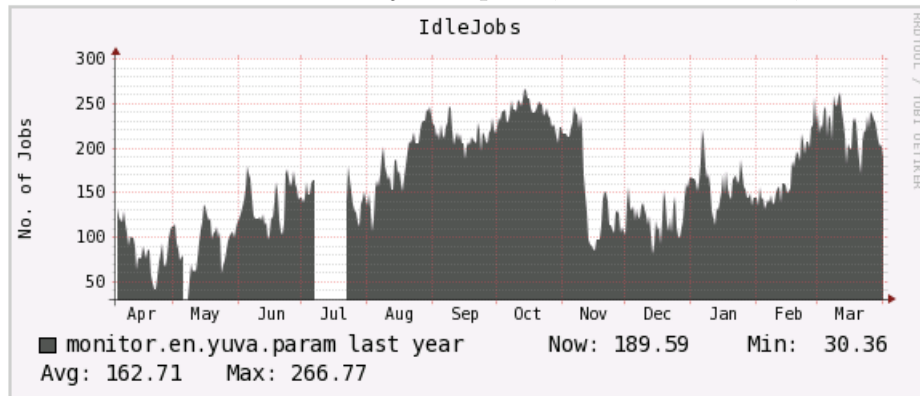
Running Jobs (Active Jobs)

PARAM Yuva II - Active jobs April 1, 2015 - March 31, 2016



Idle Jobs (Jobs waiting in queue to start running)

PARAM Yuva II - Idle jobs April 1, 2015 - March 31, 2016

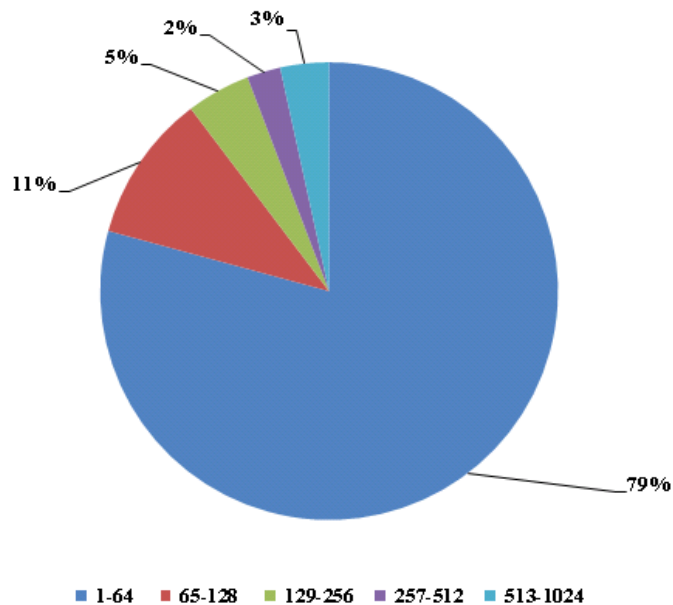


From the figures above, we see that about 100 jobs are running and equal number of jobs are always in queue waiting for their turn to start running. This indicates the need for more resources.

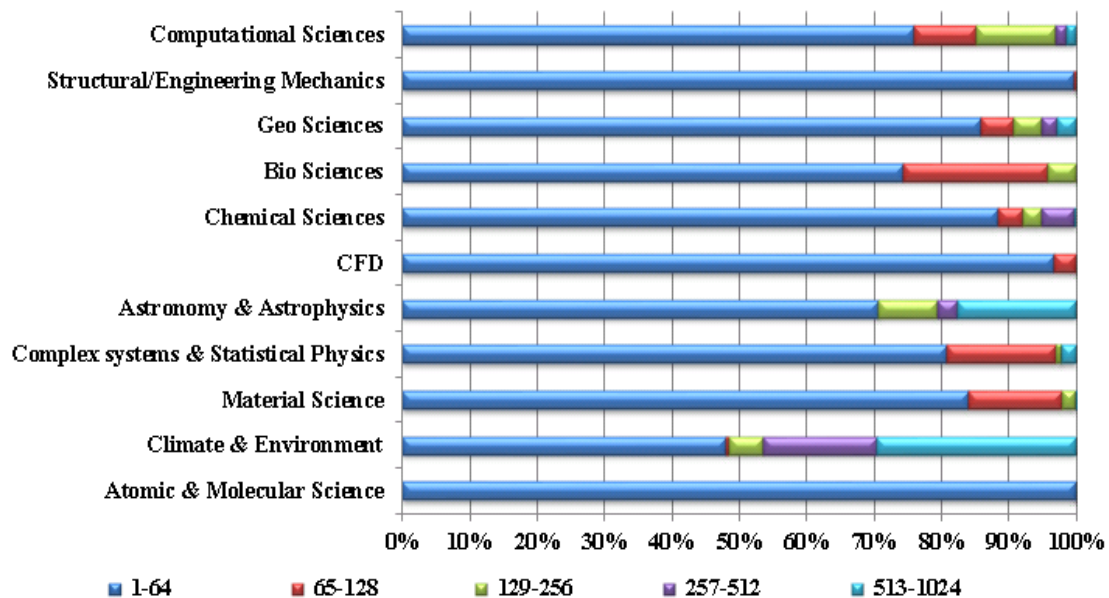
There was a partial shutdown of PARAM Yuva II (some of the nodes) from August to November due to issues related to power and cooling infrastructure. The partial shutdown during this period is reflected as the increase in the number of jobs in the queue, waiting for their turn to start running.

CPU Utilization (Period: April 1, 2015 - March 31, 2016)

CPU Time utilization vs no. of cores



Job Size (CPU cores) across application domains

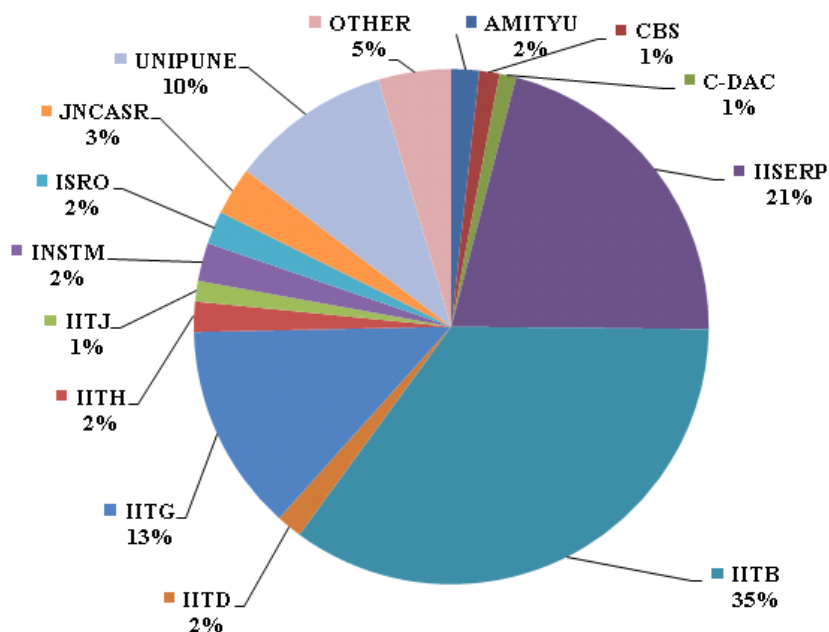


9 Jobs used more than 1024 cores.

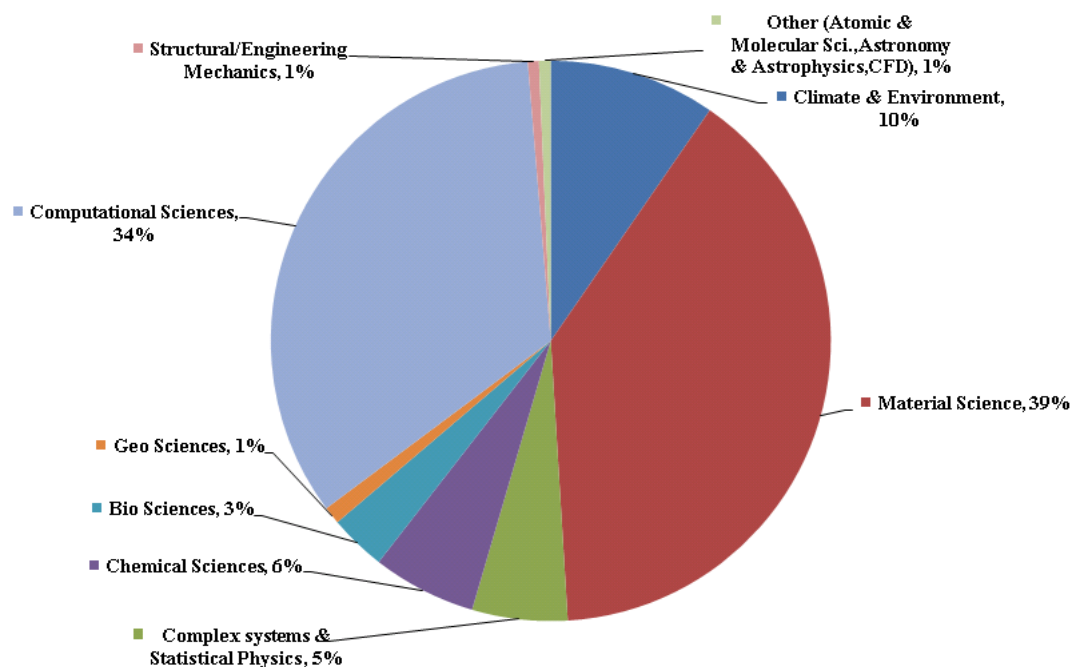
Home grown code of Seismic data processing group,C-DAC, Pune, has scaled upto 2496 cores of PARAM Yuva II.

CPU Utilization (Period: April 1, 2015 - March 31, 2016)

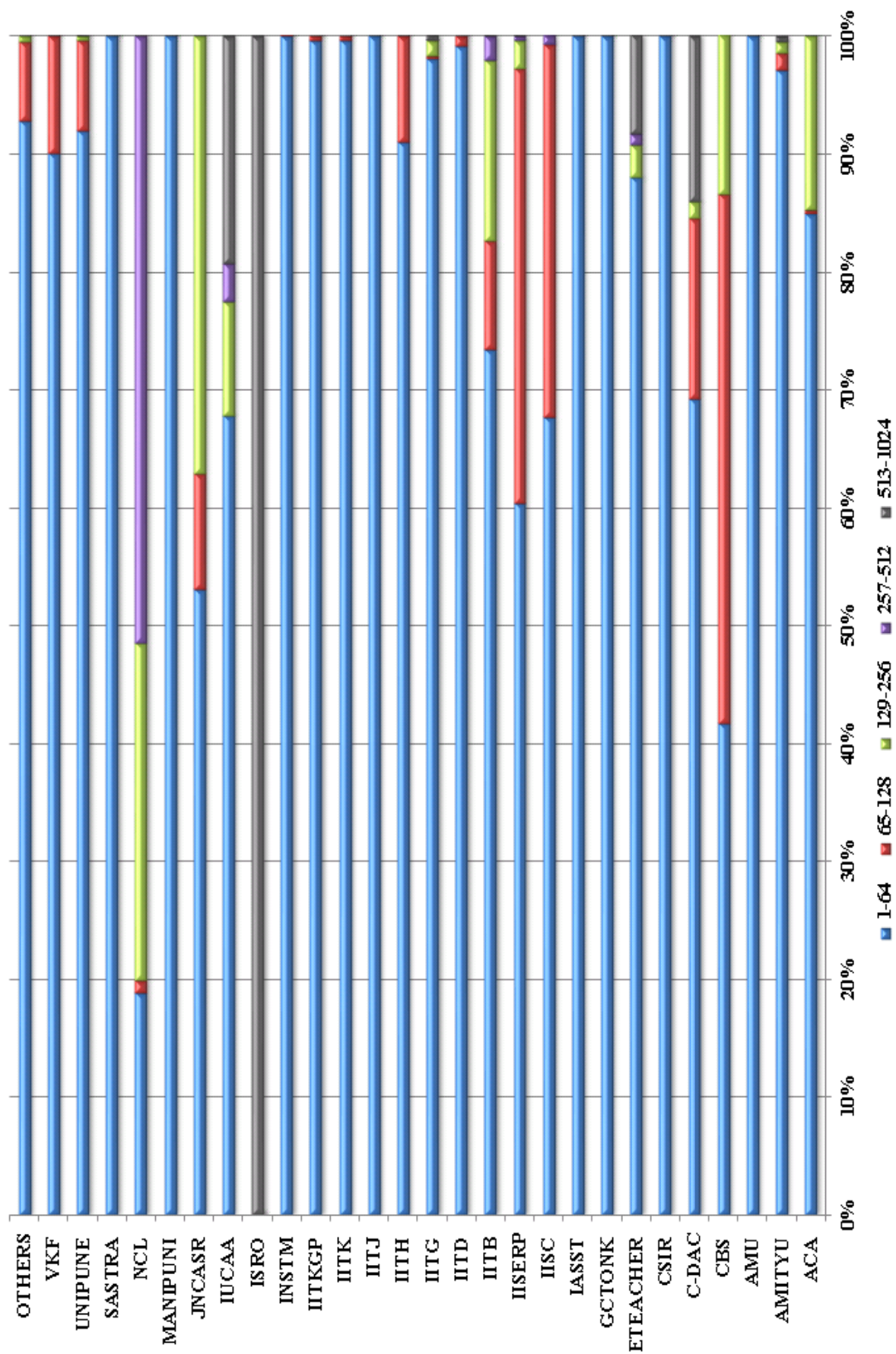
Institute wise CPU utilization in (%)



CPU time utilization in (%) across application domains



Job Statistics (Period: April 1, 2015 - March 31, 2016)



All Users:

Number of Jobs = 48,094 (Period: April 1, 2015 - March 31, 2016)

Total Number of Jobs = 1,92,708 (Period: February 19, 2013 - March 31, 2016)

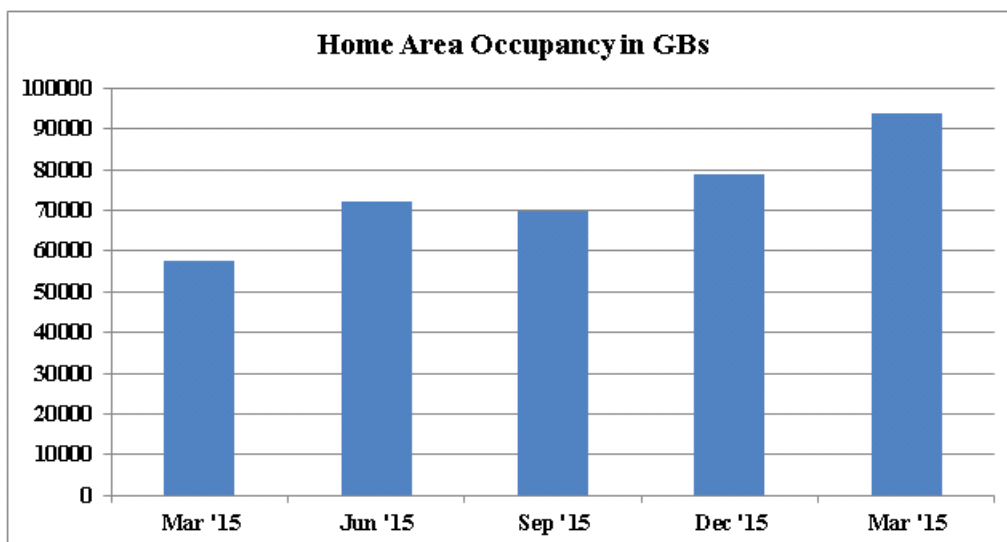
Jobs across Domains

Table 5.3: Jobs across Domains

Domain	Jobs
Atomic & Molecular Science	228
Climate & Environment	4734
Material Science	24231
Complex systems & Statistical Physics	1432
Astronomy & Astrophysics	34
CFD	791
Chemical Sciences	2066
Bio Sciences	1033
Geo Sciences	1359
Structural/Engineering Mechanics	1340
Computational Sciences	10846
Total	48094

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 (added/modified) are shown in the plots below.



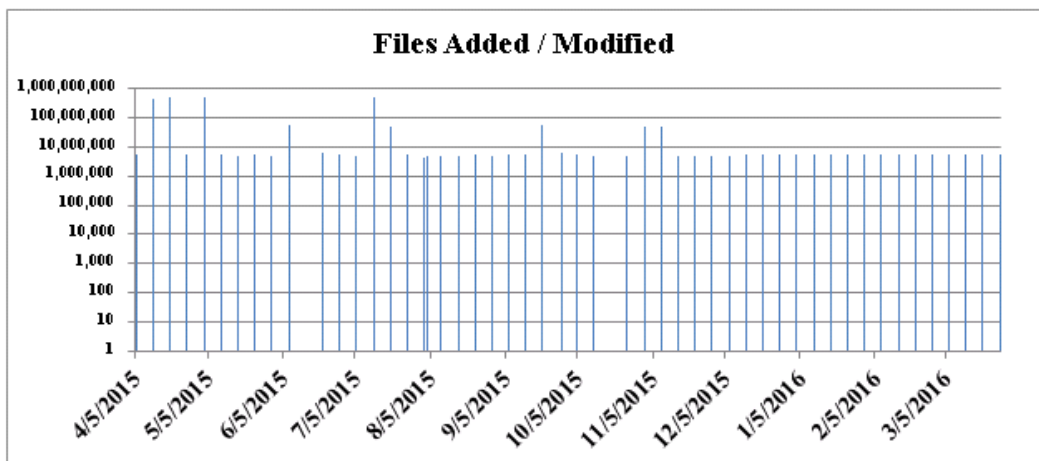
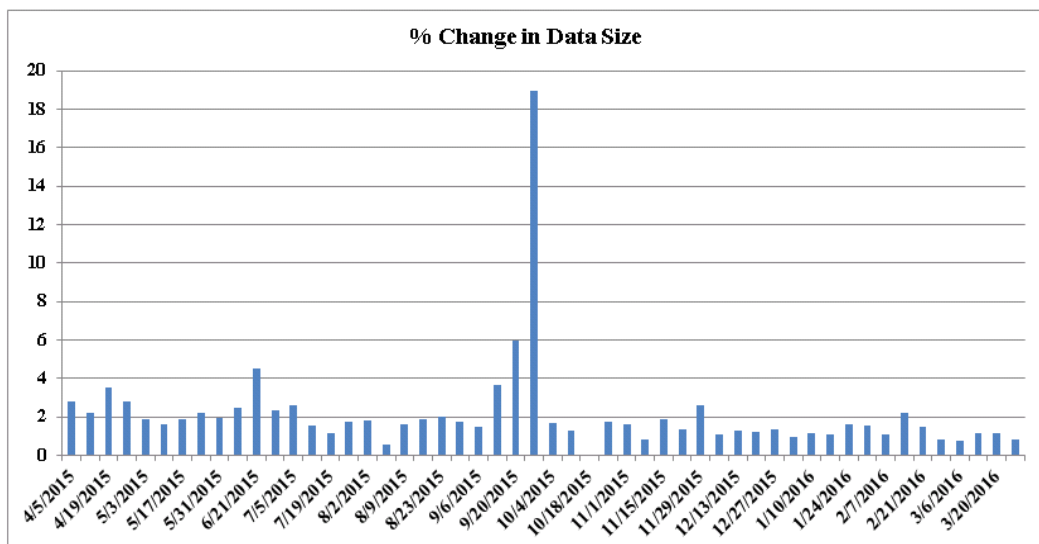
Every user of PARAM YuvaII has a storage quota allocated. Total of such quota allocations was reached 96 % of the available storage space. In order to reduce the storage

allocations, the quota of the inactive users was reduced to a minimum value (slightly greater than individual home area occupancy) and now the quota allocations has reached 176.78 TB which is 89.51 % of the total available storage space. This is an indicator for the 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. Also it is to be noted that most of the user files in the home area are the small files, however it is the large files which constitutes the majority of the storage capacity usage. The storage is divided into home area and high performance scratch area as mentioned in the compute resources. It has been observed that about 8000 (16.6 %) of the jobs have used the scratch area available for data staging

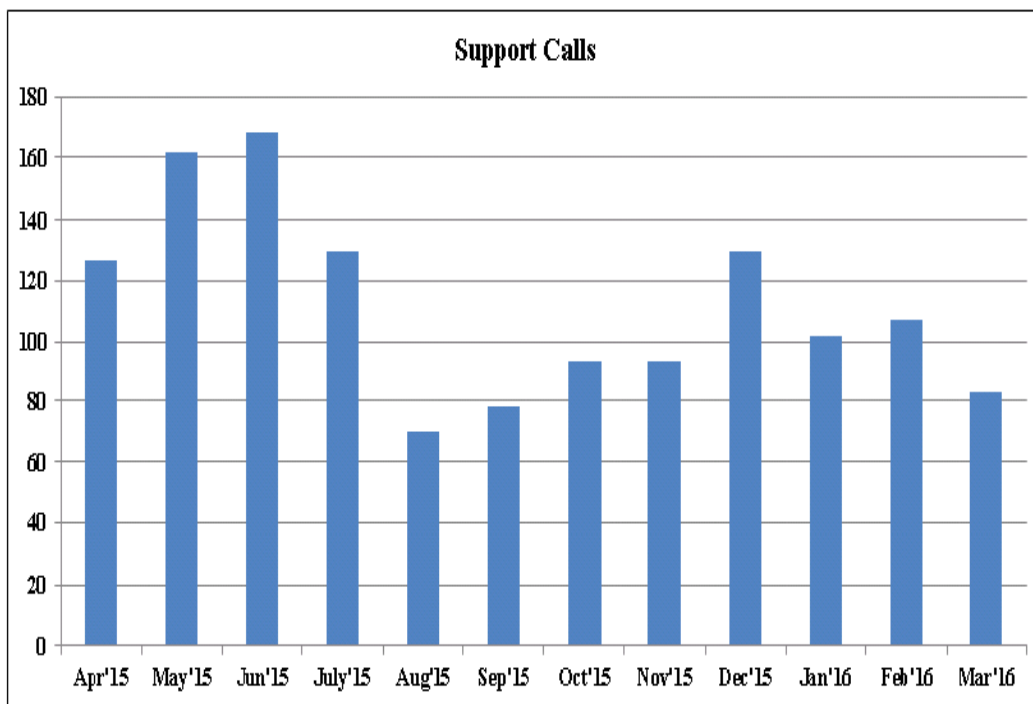
Table 5.4: Variation of home area in the storage.

Date	Size (in TB)	No. of files
13 Oct. 2015	83.37	61,14,1736
31 Mar. 2016	94	13,02,66,928



User Support Calls:

The NPSF-Help team handles about 112 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.



In FY 2015-16 : User's added : 123 ; Institution added : 16 ; Jobs Processed : 48094
% of max. cores(513-1024 cores) used by Climate & Environment application domain

6

Resources Allocation Program

The allocation program named 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 well in advance in order to ensure fairness across the user community in availing the slots under DSBF. The users are expected to submit a detailed report of the utilization of the slot and the activity carried out in the given format.

These slots are 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 interrupted job at a later point of time. The request for immediate resources from users were accommodated 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 brought under the purview of DSBF.

The table^{**} 6.1 gives a summary of the slots under DSBF during 2015-16.

[¶]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 6.1: Summary of the utilization of dedicated slots

User	Chief Investigator	Institution	Domain	Start Time	Duration	#Nodes
2016						
Mr. Ankit Mahato	Mr. Ankit Mahato	IIT Kanpur	Comp. Sc.	2016-03-11 12:00:00:0	2:12:0:0	2
Mr. Ankit Mahato	Mr. Ankit Mahato	IIT Kanpur	Comp. Sc.	2016-03-07 10:00:00:0	4:7:12:0	1
Mr. Sagar Khavnekar	Dr. Avinash Kale	CBS Mumbai	Bio Sc.	2016-02-29 18:00:00:0	7:0:0:0	64
Mr. Sagar Khavnekar	Dr. Avinash Kale	CBS Mumbai	Bio Sc.	2016-02-22 18:00:00:0	7:0:0:0	64
Ms. Richa Rastogi	Ms. Richa Rastogi	C-DAC Pune	Geo Sc.	2016-02-22 12:00:00:0	0:4:0:0	156
Ms. Richa Rastogi	Ms. Richa Rastogi	C-DAC Pune	Geo Sc.	2016-02-22 16:00:00:0	0:5:0:0	128
Mr. Subrahmanyam S	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2016-02-15 18:00:00:0	7:0:0:0	64
Ms. Tanmaya Karmarkar	Ms. Tanmaya Karmarkar	E-teacher	Comp. Sc.	2016-02-15 00:00:00:0	7:12:0:0	1
Mr. Rohit Babar	Dr. Mukul Kabir	IISER Pune	Material Sc.	2016-02-08 18:00:00:0	7:0:0:0	64
Mr. Debashish Das	Dr. Subhradip Ghosh	IIT Guwahati	Material Sc.	2016-02-01 18:00:00:0	7:0:0:0	64
Ms. Tanmaya Karmarkar	Ms. Tanmaya Karmarkar	E-teacher	Comp. Sc.	2016-01-25 0:8:55:0	38:9:50:0	4
Mr. Ashis Kundu	Dr. Subhradip Ghosh	IIT Guwahati	Material Sc.	2016-01-25 18:00:00:0	7:0:0:0	64
Mr. Chandan Kr. Singh	Dr. Mukul Kabir	IISER Pune	Material Sc.	2016-01-18 18:00:00:0	7:0:0:0	64
Mr. Yogeshwar Ajjugal	Dr. R. Thenmalarchelvi	IIT Hyderabad	Bio Sc.	2016-01-11 18:00:00:0	7:0:0:0	64
2015						
Ms. Tanmaya Karmarkar	Ms. Tanmaya Karmarkar	E-teacher	Comp. Sc.	2015-12-31 20:30:00:0	0:3:30:0	4
Mr. Abhishek Srivastav	Ms. Richa Rastogi	C-DAC	Geo Sc.	2015-12-17 18:00:00:0	0:12:0:0	64
Dr. Sandeep K. Joshi	Dr. Sandeep K. Joshi	C-DAC	Comp. Sc.	2015-09-02 18:00:00:0	0:15:50:0	64
Dr. Sandeep K. Joshi	Dr. Sandeep K. Joshi	C-DAC	Comp. Sc.	2015-09-01 18:00:00:0	0:15:50:0	64
Mr. Vaibhav Kaware	Dr. Kavita Joshi	NCL Pune	Chemical Sc.	2015-06-15 17:00:00:0	7:0:0:0	64
Mr. Subrahmanyam S	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2015-06-08 17:00:00:0	7:0:0:0	64
Mr. Subrahmanyam S	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2015-06-01 17:00:00:0	7:0:0:0	64

Continued on next page

Table 6.1 – Continued from previous page

User	Chief Investigator	Institution	Domain	Start Time	Duration	# Nodes
Prof. Shridhar R. Gadre	Prof. Shridhar R. Gadre	IIT Kanpur	Chemical Sc.	2015-05-25 17:00:00:0	7:0:0:0	64
Mr. Sangkha Bora	Dr. P. Padma Kumar	IIT Guwahati	Chemical Sc.	2015-05-18 17:00:00:0	7:0:0:0	64
Dr. Arnab Mukherjee	Dr. Arnab Mukherjee	IISER Pune	Bio Sc.	2015-05-11 17:00:00:0	7:0:0:0	64
Dr. Anjali Kshirsagar	Dr. Anjali Kshirsagar	S. P. UniPune	Material Sc.	2015-05-04 17:00:00:0	7:0:0:0	64
Dr. R. Thenmalarchelvi	Dr. R. Thenmalarchelvi	IIT Hyderabad	Bio Sc.	2015-04-27 17:00:00:0	7:0:0:0	64
Mr. Ashis Kundu	Dr. Subhradip Ghosh	IIT Guwahati	Material Sc.	2015-04-20 17:00:00:0	7:0:0:0	64
Mr. Ashis Kundu	Dr. Subhradip Ghosh	IIT Guwahati	Material Sc.	2015-04-13 17:00:00:0	7:0:0:0	64
Mr. Nandha Kumar	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2015-04-06 17:00:00:0	7:0:0:0	64
Mr. Nandha Kumar	Dr. Prasenjit Ghosh	IISER Pune	Material Sc.	2015-03-30 17:00:00:0	7:0:0:0	64

Total dedicated slots in FY 2015-16 : 30

7

Major Research Projects

This is the list of major research projects^{††} based on the research publication/s in high impact journals from the work that has been carried out on PARAM Yuva II.

Structure and dynamics of RMA duplexes comprising trinucleotide repeat expansion

Dr. Thenmalarchelvi Rathinavelan, IIT, Hyderabad

Ab initio Molecular Dynamics simulation of Ionic Liquid doped Polymer Electrolyte Membranes and Platinum Electrode Interface

Dr. Anurag Prakash Sunda, Pandit Deendayal Upadhyay Shekhawati University, Sikar, Rajasthan

Electronic structure calculations of semiconductor

Prof. S. V. Ghaisas, S. P. Pune Pune University, Pune

Multiscale simulation of shear of micellar systems

Dr. Apratim Chatterji, IISER, Pune

Chalcogenides nanostructures for catalytic and electrochemical applications

Dr. P Murugan, CSIR-Central Electrochemical Research Institute, Karaikudi, Tamil Nadu

Research work on nano-materials

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

Quantum chemical studies on understanding the interactions of molecules and molecular clusters with graphyne and graphdiyne

Dr. R. S. Swathi, IISER, Thiruvananthapuram

Electronic structure and scattering dynamics

Dr. Aditya Panda, IIT, Guwahati

Materials Modelling at Different Length and Time Scales

Dr. Mukul Kabir, IISER, Pune

Study of Structural, Electronic and Magnetic Properties of Nanomaterials

Dr. Mrinalini Deshpande, HPT Arts and RYK Science College, Nasik

^{††}Please refer Appendix A for the complete list of projects.

8

Ph.D Theses by PARAM Yuva II Users

1. **Transversal Pattern Formation in Shallow Non-adiabatic Packed Bed Reactors** (April, 2015)
Student: Mr. K. Narendiran, Dept. of Chemical Engineering, IIT, Bombay
Supervisor: Prof. Ganesh A. Viswanthan
2. **Ab-initio study of undoped silicon nanoclusters and graphene for magnetic properties- Role of vacancies** (June, 2015)
Student: Ms. Priya Francis, Dept. of Electronic Science, S. P. Pune University
Supervisor: Prof. S. V. Ghaisas,
3. **Electronic Structure and Optical Properties of pi-conjugated Systems: Oligoacenes and Trigonal Zigzag Graphene Nanodisks** (July, 2015)
Student: Ms. Himanshu Chakraborty, Dept. of Physics, IIT, Bombay
Supervisor: Prof. Alok Shukla
4. **Theoretical Studies of atomic and electronic structure of metal doped semiconductor clusters and their vibrational Properties** (August, 2015)
Student: Ms. Stuti Jaiswal, VKF, Gurgaon and Sunrise University, Alwar, Rajasthan
Supervisor: Prof. Vijay Kumar (VKF, Gurgaon)
5. **Ab-initio calculations for determining the diffusion barriers for Cd,Te and Sulfur on CdTe <111>surface** (September, 2015)
Student: Ebadollah Naderi, Dept. of Physics, S. P. Pune University
Supervisor: Prof. S. V. Ghaisas, Dept. of Electronic Science
6. **Electronic, structural and finite temperature studies of nano structured materials using ab-initio methods** (03 September, 2015)
Student: Mr. Vaibhav Kaware, S. P. Pune University, Pune
Supervisor: Prof. D.G. Kanhere and Prof. Anjali Kshirsagar
7. **Protein thermal stability, conformational dynamics and solvent properties: insights with atomistic molecular dynamics simulations** (October, 2015)
Student: Mr. Prathit Chatterjee, National Chemical Laboratory, Pune
Supervisor: Dr. Neelanjana Sengupta
8. **Evaluation of TanDEM-X interferometric digital elevation models obtained over various terrains** (October/November, 2015)

Student: Ms. Rinki Deo, Centre for Studies in Resource Engineering, IIT, Bombay
Supervisor: Prof. Y. S. Rao

9. **DNS studies of the boundary layer on a low pressure turbine blade at high incidence** (27 November, 2015)

Student: Mr Rajesh Ranjan, Engineering Mechanics Unit, JNCASR, Bangalore
Supervisor: Prof. Roddam Narasimha

10. **Developments of Algorithms for Accurate Energetics and Spectra of Molecular Aggregates within Fragmentation Approach** (11 January, 2016)

Student : Nityananda Sahu, S. P. Pune University, Pune
Supervisor : Professor Shridhar R. Gadre

11. **Atomistic investigation of polymer electrolyte membrane nanostructure and dynamics of molecular transport in fuel cells** (January, 2014)

Student: Mr. Anurag P. Sunda, Dept. of Chemistry, IISER, Pune
Supervisor: Prof. Arun Venkatanathan

12. **Ab initio Calculations of Optical Properties of Clusters** (June, 2014)

Student: Mr. Ravindra L. Shinde, Dept. of Physics, IIT, Bombay
Supervisor: Prof. Alok Shukla

9

Science using PARAM Yuva II

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.

Nucleic Acids Research (9.112)

Bharathi Reddy Kunduru, Sanjana Anilkumar Nair and Thenmalarchelvi Rathinavelan, EK3D: an E. coli K antigen 3 dimensional structure database, Nucl. Acids Res. **44** (D1), D675, (2016).

Journal of Material Chemistry (7.443)

Anurag P. Sunda, Ammonium-based Protic Ionic Liquid Doped Nafion Membrane as Anhydrous Fuel Cell Electrolyte, J. Material Chem. A **3**, 12905 (2015).

Carbon (6.196)

Priya Francis, Chiranjib Majumder and S. V. Ghaisas, The nonchalant magnetic moment in Graphene, Carbon **91**, 358 (2015).

Macromolecules (5.8)

Amruta Kulkarni, Ashish Lele, Swaminathan Sivaram, P. R. Rajamohanan, Sachin Velankar and Apratim Chatterji, Star Telechelic Poly(l-lactide) Ionomers, Macromolecules **48**(18), 6580 (2015).

Journal of Physical Chemistry C (4.772)

J. Karthikeyan, V. Kumar and P. Murugan, The Role of Valence Electron Concentration in Tuning the Structure, Stability, and Electronic Properties of Mo6S 9-xIx Nanowires, J.

Phys. Chem. C **119**, 13979 (2015).

Bheema Lingam Chittari and Vijay Kumar, Ab Initio Studies of Segregation, Ordering, and Magnetic Behavior in (Fe-Pt)_n, n = 55 and 147: Design of Fe₇₅Pt₇₂ Nanoparticle. J. Phys. Chem. C **119**, 11062 (2015).

S. Chandra Shekar and R. S. Swathi, Cation Interactions and Rattling Motion through Two-Dimensional Carbon Networks: Graphene vs Graphynes, J. Phys. Chem. C **119**, 8912 (2015).

Harikrishna Sahu and Aditya N. Panda, Helical and Non-helical Structures of Vinylene-and Azomethine-linked Heterocyclic Oligomers: A Computational Study of Conformation-dependent Optoelectronic Properties, J. Phys. Chem. C **119**(40), 22855 (2015).

Mukul Kabir, and Krystyn J Van Vliet, Kinetics of Topological Stone-Wales Defect Formation in Single Walled Carbon Nanotubes, J. Phys. Chem. C , (2015). (*Accepted*)

Physical Chemistry Chemical Physics (4.493)

Manasi S. Mahabal, Mrinalini D. Deshpande, Tanveer Hussain and Rajeev Ahuja, Sensing Characteristics of a Graphene-like Boron Carbide Monolayer towards Selected Toxic Gases, Phys. Chem. Chem. Phys. **16**, 3551 (2015).

Journal of Nanostructure in Chemistry (3.84)

S. Chopra and Rai, B., DFT/TDDFT study of electronic and optical properties of Surface passivated Silicon nanocrystals, Sin (n = 20, 24, 26 and 28) , J. Nanostruct. Chem., **5**, 195 (2015).

Physical Review B (3.736)

Bheema Lingam Chittari and V. Kumar, Atomic structure, alloying behaviour, and magnetism in small Fe-Pt clusters, Phys. Rev. B (2015). (*Accepted*)

Deepika, T. J. Dhilip Kumar, Alok Shukla and Rakesh Kumar, Edge configurational effect on band gaps in graphene nanoribbons, Phys. Rev. B **91**, 115428 (2015).

T. Basak, H. Chakraborty, and A. Shukla, Theory of linear optical absorption in diamond shaped graphene quantum dots, Phys. Rev. B **92**, 205404 (2015).

Chemical Physics and Physical Chemistry (3.419)

S. Chopra, Study of electronic, optical absorption and emission in pure and metal decorated Graphene nanoribbons (C₂₉H₁₄-X): First principles calculations, ChemPhysChem. **16**(9), 1948 (2015).

Kulkarni, M. and Mukherjee A., Computational Approach to Explore the B/A Junction Free Energy in DNA, ChemPhysChem **17**(1), 147 (2016).

Journal of Physical Chemistry B (3.302)

Subrata Paul and Sandip Paul, Exploring the Counteracting Mechanism of Trehalose on Urea Conferred Protein Denaturation: A Molecular Dynamics Simulation Study, *J. Phys. Chem. B* **119**, 9820 (2015).

Bhanita Sharma and Sandip Paul, Understanding the Role of Temperature Change and the Presence of NaCl salts on Caffeine Aggregation in Aqueous Solution: From Structural and Thermodynamics Point of View, *J. Phys. Chem. B* **119**, 6421 (2015).

Subrata Paul and Sandip Paul, Mechanism of Hydrotropic Action of Hydrotrope Sodium Cumene Sulfonate on the Solubility of Di-*t*-Butyl-Methane: A Molecular Dynamics Simulation Study, *J. Phys. Chem. B* **120**(1), 173 (2016).

K. R. Ramya, Praveen Kumar and A. Venkatnathan, Molecular Simulations of Anion and Temperature Dependence on Structure and Dynamics of 1-hexyl-3-methylimidazolium Ionic Liquids, *J. Phys. Chem. B* **119**, 14800 (2015).

New Journal of Chemistry (3.086)

M. M. Deshmukh, S. R. Gadre and E. J. Cocinero, Stability of Conformationally Locked Free Fructose: Theoretical and Computational Insights, *New J. Chem.* (2015). (*Accepted*)

Journal of Chemical Physics (2.952)

Nalini Gurav, Anant Kulkarni, Shridhar Gejji, and Rajeev Pathak, CH₃OH...(H₂O)_n [n=1-4] clusters in external electric fields, *J. Chem. Phys.* **142**, 214309 (2015).

Journal of Physics D (2.721)

Debashish Das and Subhradip Ghosh, Density Functional Theory based comparative study of electronic structure and magnetic properties of ACr₂O₄ (A=Mn,Fe,Co,Ni) compounds. *J. Phy. D: Applied Physics* **48**, 425001 (2015).

Journal of Physical Chemistry A (2.693)

S. S. Rao, N. B. Bejoy and S. P. Gejji. Hydrogen Bonding, ¹H NMR and Molecular Electron Density Topographical Characteristics of Ionic Liquids Based on Amino Acid Cations and Their Ester Derivatives. *J. Phys. Chem. A* **119**, 8752 (2015).

Gurmeet Singh, Rahul Verma and Shridhar R Gadre, Understanding Packing Patterns in Crystals by Analysis of SmallAggregates: A Case study of CS₂, *J. Phys. Chem. A* **119**, 13055 (2015).

Journal of the American Ceramic Society (2.610)

K. Ganga Prasad, Manish K. Niranjana, Saket Asthana, and R. Karthikeyan, Investigation of Raman Modes and Born-Effective Charges in AgNb_{1/2}Ta_{1/2}O₃: A Density-Functional

and Raman Scattering Study, J. Am. Ceram. Soc. **99**(1), 1 (2015).

Amol B. Rahane, Vijay Kumar, and Jennifer S. Dunn, Carbon Doping in Boron Suboxide: Structure, Energetics, and Elastic Properties. J. Am. Ceram. Soc. **98**, 2223 (2015).

Industrial & Engineering Chemistry Research (2.587)

K. Narendiran, and G. A. Viswanathan, Impact of Wall Heat Transport on Formation of Transversal Hot Zones in Shallow, Non-adiabatic Packed-Bed Reactors, Ind. Eng. Chem. Res. **54**, 7352 (2015).

Journal of Molecular Liquids (2.515)

Subrata Paul and Sandip Paul, Influence of Temperature on the Solvation of N-methylacetamide in Aqueous Trehalose Solution: A Molecular Dynamics Simulation Study, J. Mol. Liq. **211**, 986 (2015).

P. L. Verma, S. S. Rao and S. P. Gejji, Probing Molecular Interactions Underlying Imadazolium and Pyridinium based Ionic Liquids., J. Mol. Liq. **212**, 885 (2015).

S. S. Rao, D. N. Lande and S. P. Gejji, Density functional theory investigations on binding and spectral features of complexes of ferrocenyl derivatives with cucurbit [7]uril, J. Mol. Liq. **216**, 309 (2016).

M. N. Shewale, D. N. Lande and S. P. Gejji, Encapsulation of benzimidazole derivatives within cucurbit[7]uril: density functional investigations, J. Mol. Liq. **216**, 298 (2016).

Boundary-Layer Meteorology (2.47)

Prashant Kumar, Bimal K. Bhattacharya, and P. K. Pal, Evaluation of Weather Research and Forecasting Model Predictions Using Micrometeorological Tower Observations, Boundary-Layer Meteorology (2015). (*Accepted*)

Journal of Physics: Condensed Matter (2.346)

Vikas Kashid, Vaishali Shah, H. G. Salunke, Y. Mokrousov and, S. Bluegel, Magnetic properties of 2D nickel nanostrips: structure dependent magnetism and Stoner criterion, J. Phys.: Cond. Matter **27**, 316002 (2015).

Journal of Applied Physics (2.183)

Prabhsharan Kaur, S. S. Sekhon, J. M. Zavada, and Vijay Kumar. Enhanced stability of Eu in GaN nanoparticles: Effects of Si co-doping, J. App. Phys. **117**, 224301 (2015).

Bhargab Deka, Ashis Kundu, Subhradip Ghosh and A. Srinivasan, Experimental and ab initio studies of sub-lattice ordering and magnetism in Co₂Fe (Ge 1-x Si X) alloys. J. Applied Phy. **118**, 133906 (2015).

EuroPhysics Letters (2.095)

Kaustubh S. Agarwal, Rajeev K. Pathak and Yogesh N. Joglekar, Exactly solvable PT-symmetric models in two dimensions, *EPL* **112** (3), 31003 (2015).

Computers and Geoscience (2.054)

R. Rastogi, A. Srivastava, K. Khonde, K. Sirasala, A. Londhe and H. Chavhan, An efficient parallel algorithm: Poststack and prestack Kirchhoff 3D depth migration using flexi-depth iterations, *Computers & Geosciences* **80**, 1 (2015).

Theoretical and Applied Climatology (2.015)

S. Nayak, M. Mandal and S. Maity, Customization of regional climate model (RegCM4) over Indian region, *Theo. and App. Clim.*, (2015). (*Accepted*)

Surface Science (1.925)

Nandha Kumar and Prasenjit Ghosh, Structure and Stability of Clean and Adsorbate Covered Intermetallic PdGa Surfaces: A First Principles Study, *Surface Science* **644**, 69 (2016).

Pradip B. Shelke and A.V. Limaye, Dynamics of Random Sequential Adsorption (RSA) of linear chains consisting of n circular discs-Role of aspect ratio and departure from convexity. *Surface Science* **637**, 1 (2015).

Molecular Physics (1.720)

N. Sahu, S. S. Khire and S. R. Gadre, Structures, Energetics and Vibrational Spectra of (H₂O)₃₂ Clusters: A Journey from Model Potentials to Correlated Theory, *Mol. Phys.* (2015). (*Accepted*)

Materials Research Express (1.647)

Manish K. Niranjana, Anisotropy in elastic properties of TiSi₂ (C49, C40 and C54), TiSi and Ti₅Si₃: an ab-initio density functional study, *Mater. Res. Express* **2**, 096302 (2015).

Computational and Theoretical Chemistry (1.545)

S. Rao and S. P. Gejji, Molecular Insights Accompanying Aggregation in Amino Acid Ionic Liquids. *Comp. Theor. Chem.* **1057**, 24 (2015).

Molecular Simulation (1.133)

Gopal Kandhakumar, Mailsamy Jothi and Poomani Kumaradhas, Probing the effect of nitro groups in nitramine based energetic molecules: a DFT and Charge density study, *Mol. Simulation* **42**(3), 173 (2015).

Canadian Journal of Chemistry (1.061)

G. Kandhakumar, C. Kalaiarasi and P. Kumaradhas, Structure and charge density distribution of amine-azide based hypergolic propellant molecules: A Theoretical Study, Canadian J. of Chem. (2016). (*Accepted*)

Particulate Science and Technology (0.523)

K. Naval, K. Gopee, B. Manaswita, Transition Criteria for Fluidized Beds Revisited, Particulate Sci. and Tech. **33**(4), 393 (2015).

International Journal of Applied Engineering and Technology (0.302)

V. Sivakumar and A. Goyal, Geospatial Information Extraction from Multispectral Satellite Imagery through GPU'S based Parallel Computation Approach, Int. J. of App. Engg. and Tech. **4**, 61 (2014).

Conference Proceedings

Aditya A. Gupte, A.M. Pradeep, and P.M. Mujumdar, Numerical Analysis of Synthetic Jet in Crossflow, 22nd AIAA Computational Fluid Dynamics Conference, June 2015.

Nilesh Maltare, Experiment to exploit parallelism by Parallel Design Patterns on MPI cluster, ACM Conference PDPTA'15, Nevada USA: The 2015 International Conference on Parallel and Distributed Processing Techniques and Applications. (*Accepted*)

K. Naval and B. Manaswita, CFD-DEM simulations for gas solid flow in a fluidized bed, APCCChE 2015: Congress incorporating Chemeca 2015, Melbourne, Victoria. Paper no. 3135330, September-October 2015.

Naval V. Koralkar, Gopee K. Krushna, Manaswita Bose, Stability Criteria for transition from homogeneous to bubbling fluidization, PGBSIA-2013.

Mohan Labade, Vikas Kumar, and Srisai Meher, Flow simulation studies on HPC platform with GPU accelerator, 42nd National Conference on Fluid Mechanics and Fluid Power, National Institute of Technology Karnataka, Surathkal, December , 2015.

Nilesh Maltare, Generating Large Prime on MPI Cluster by applying Parallel Design Patterns, ICICT 2015 and Springer AISC Series 2015. (*Accepted*)

Vikas Kashid, Shantanu Kadam, H. G. Salunke, Anjali Kshirsagar, The structure and electronic properties of MoS 2 and WS 2 monolayer composites, DAE, Solid State Physics Symposium 2015. (*Accepted*)

Manaswita Bose, 2016, Velocity distribution of particles in low velocity pneumatic conveying systems, International Complex Fluids Conference(Compflu - 2016), IISER, Pune, India, January, 2016.

10

Visits @ PARAM Yuva II

Visits by Officials, Members of Academia & Industry

1. Dr. S. Chaudhari, Director(S&T) and Director(Admin), North Eastern Council, Ministry of Development of NE Region, Government of India (Aug. 2015).
2. Dr. Manish Jindal, Registrar, PEC University of Technology, Chandigarh (Oct. 9' 2015).
3. Mr. J. Alan Bird, Global Business Development Leader, Massachusetts Institute of Technology (MIT), Massachusetts (Feb. 04 2016).
4. Prof. Bernard Songwar, Director, India Seychelles Centre of Excellence in ICT (ISCEICT) , from Feb. 29 Mar. 2, 2016.
5. Shri S. A. Kumar, Head of High Performance Computing Division, DeitY (Mar. 10' 2016).



Shri S. A. Kumar (3rd from the left), Scientist F, Head, HPC Division, DeitY

Table 10.1: Summary of Industrial Visits for students

Institution	No. of visitors	Visit Date
2015		
Rajarshi School of Management and Technology, Varanasi	43	Apr. 01
Indian Navy	50	Apr. 23
GTU, Gujarat	15	May 21
NIT, Silchar	10	Jun. 5
Symbiosis International University	32	Jul. 22
ACTS, C-DAC, Pune	43	Jul. 24
JECRC University Jaipur	26	Aug. 13
K. J. Somaiya College of Science&Commerce, Mumbai	55	Aug. 13
D. Y. Patil College of Engineering, Talegaon	100	Aug. 17
D. Y. Patil Institute, Management and Research, Akurdi	62	Aug. 17
AISSMS, Pune	75	Aug. 21
Smt. S. H. Mansukhani Institute of Technology, Ulhasnagar	105	Aug. 21
Sree Chithrathirunnal College of Engineering, Trivandrum	52	Aug. 25
Marwadi Education foundation, Rajkot	31	Sep. 2
M.H. Saboo Siddik College of Engineering, Byculla, Mumbai	30	Sep. 4
MGM Polytechnic, Aurangabad	46	Sep. 4
K J Institute of Technology and Management, Vadodara	53	Sep. 14
R. J. College of Arts, Science & Commerce, Mumbai	58	Sep. 18
e-Procurement training	35	Sep. 30
S. H. Jondhale Polytechnic, Thane	60	Oct. 12
Bharati Vidyapeeth Institute of Technology	54	Oct. 15
ASM's Institute of Business Management and Research, Pune	100	Oct. 16
Banasthali Vidyapeeth, Rajasthan	15	Nov. 4
College of Engineering, Pune	18	Nov. 6
2016		
Bharat College of Arts and Commerce, Thane	44	Jan. 12
Accelerating Biology, C-DAC	250	Jan. 19
Kalsekar College, Thane	50	Jan. 21
AISSMS, Pune	6	Jan. 27
D-ITSS, ACTS	40	Jan. 28
Latthe Polytechnic, Sangli	33	Feb. 2
Sarvajanic College of Engineering and Technology, Surat	37	Feb. 5
PICT, Pune	44	Feb. 11
Vivekanand Science College, Buldhana	103	Feb. 12
VAMNICOM, Pune	30	Feb. 18
Dr.D.Y.Patil Polytechnic,Kolhapur	40	Feb. 28
Babaria Institute of Technology, Vadodara	90	Feb. 28
COEP, Pune	20	Mar. 9
PG-DBDA,ACTS	20	Mar. 10
D.Y. Patil Polytechnic,Talsande, Kolhapur	41	Mar. 18
PES College of Engineering, Aurangabad	35	Mar. 28

Total number of PARAM Yuva II visitors in FY 2015-16 : 2051

Appendix A

Projects @ PARAM Yuva II

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
Ahmednagar College	Investigation of semiconducting nano clusters using first principle calculations	Dr. Pardip Shelke	1
Aligarh Muslim University	Higher Order calculations in Field Theory	Dr. Abbas Ali	5
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
BITS-Pilani Hyderabad	Computational Fluid Dynamics based Process Modeling, Optimization and Scale-up of Flotation Cell	Dr. Jeevan Jaidi	2
CBS, Mumbai	Conformational dynamics of actin and its regulators	Dr. Avinash Kale	2
CIFRI, Kolkata	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. Varahabatra Narayana	2
Carnegie Mellon University	Adsorption of ionic liquids on graphene surface	Dr. Niles R. Dhumal	1
CECRI, Karaikudi	Metal chalcogenides nanostructures for catalytic and electrochemical applications	Dr. P. Murugan	1
	Finite Temperature Behaviour of atomic clusters and nano-carbon materials	Dr. Sailaja Krishnamurthy	3

Continued on next page

Table A.1 – Continued from previous page

Institution	Project	Chief Investigator	No. of Users
Central Univ. of Bihar	Molecular Dynamics study of thermo-stability of archaeal 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
COEP, Pune	Flow around a bundle of square cylinder	Dr. C. M. Sewatkar	2
Delhi University	MD Simulations project of Delhi University	Prof. Parbati Biswas	2
E-Teacher	HPC Program Analysis a representation tools to provide Backend for an on-line Engineering E-teacher	Dr. Narendra Karmarkar	4
GLA university, Mathura	Theoretical investigation of novel materials applications in the field of electronics and optoelectronic devices	Dr. Bramha Prasad Pandey	1
Govt. College, Tonk	Study of P- and P, T- odd effects in heavy polar diatomics	Dr. Manu Sikarwar	1
Gurunanak Dev University	To study the atomic and electronic structure of III-V semiconductor nanostructures	Prof. S. S. Sekhon	1
Gujarat Tech. University, Ahmedabad	Adaptive Parallel Design Pattern for Multicore	Mr. Nilesh Maltare	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
	Electronic Properties of TM doped ZnO Sheet: Density Functional Study	Dr Mrinalini Deshpande	3
IASST, Guwahati	Ab initio calculations of shape memory heusler alloys	Dr. Munima B. Sahariah	3

Continued on next page

Table A.1 – Continued from previous page

Institution	Project	Chief Investigator	No. of Users
	New n-type organic semiconductors for optoelectronics: Synthesis, characterization and device fabrication	Dr. Sagar Sharma	1
IIA, Bangalore	Computational many body theory of atoms and molecules	Prof. Bhanu Pratap Das	10
	Numerical simulations of Hydromagnetic turbulence from galaxies to Sun	Dr. Sharanya Sur	2
IIT, Delhi	Explore the benefit of deep neural network for various tasks related to egocentric videos	Dr. Chetan Arora	4
IIT, Hyderabad	Simulation of Fault Motion Analysis, Simulation of Collapse behavior of buildings subjected to Earthquakes	Dr. Ramacharala Pradeep Kumar	3
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 micellar 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 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
	Computing translocation time of polypeptides using milestoning Research	Dr. Srabanti Chaudhury	2
	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
	O ₂ molecule splitting and diffusion on LaMnO ₃ surface	Dr. Mukul Kabir	3
	Quantum chemical calculations of the energetics and vibrational frequencies of non-covalently bonded aromatic complexes relevant to biology and materials	Dr. Alok Das	4
	Covering Arrays and Software Testing	Dr. Soumen Maity	3
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

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Table A.1 – Continued from previous page

Institution	Project	Chief Investigator	No. of Users
IIT Bhubaneswar	Aerodynamic characterization of natural laminar flow	Dr. Yogesh G. Bhumkar	2
IIT Bombay	High Performance Computing initiative	Prof. Amitabh Bhattacharya	150
	Development 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
	Uncertainty quantification towards improving the parameterizations for precipitation scavenging of aerosols in a General Circulation Model	Dr. Dilip Ganguly	3
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
	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
	Application of smooth exterior scaling method	Prof. Ashish Kumar Gupta	2
	Computational studies of allosteric mechanism of SAMHD1	Dr. Swati Bhattacharya	2

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Table A.1 – Continued from previous page

Institution	Project	Chief Investigator	No. of Users
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
	First Principle study of Surfaces and Interfaces	Dr. Manish Kumar Niranjan	3
IIT Jodhpur	Investigating seismic source physics inclusion into Engineering analysis of Built-Environment	Dr. Surendra Nadh Somala	2
	Magnetic functionalization and magnetotransport properties of graphene	Dr. Ambesh Dixit	1
	Theoretical study on lithium ion batteries	Dr. Ambesh Dixit	2
	Chemical Dynamics Simulations of Complex Organic Reactions: Mechanistic Insights and Micro-solvation Effects	Dr. Manikandan Paranjothy	2
IIT Kanpur	Dual scale simulations of surfactant, co-surfactant, water systems	Dr. Ananya Debnath	3
	Shape and size effects of nanoparticles on the properties of polymer nanocomposites	Prof. Jayant K. Singh	5
	Magnetohydrodynamics turbulence studies of liquid metals and dynamo	Prof. Mahendra K. Verma	7
	Thunder storm simulation	Prof. Sachchidanand Tripathi	1
IIT Kharagpur	Study of complex fluid flows past bluff bodies	Prof. Sanjay Mittal	1
	Development of a Fracture and Crack Analysis Parallel Code for Composite Materials on Hybrid HPC	Dr. Rakesh Kumar M	5
	To find the interfacial strength in CNT amine epoxy composite	Prof. Baidurya Bhattacharya	4

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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. Sonmuth Roy	4
IIT Ropar	H ₂ storage and fuel cell materials for renewable energy	Dr. T. J. Dhillip 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
	Ab initio molecular dynamics (AIMD) Simulations	Dr. Md. Ehesan Ali	1
	Electronics and Thermal Properties of chalcogenide	Dr. Chandan Bera	2
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

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Table A.1 – Continued from previous page

Institution	Project	Chief Investigator	No. of Users
	Study DDSCAT MPI Code for studying the effects of light scattering with dust in astrophysical env.	Prof. Ranjan Gupta	2
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
	Density Functional theory studies of nanosystems	Prof. Shobhana Narasimhan	2
	Studies of micro and nanoscale flows	Dr. Nandu Gopan	1
JNU	Entropy 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 transcripts to identify SNP markers 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

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Table A.1 – Continued from previous page

Institution	Project	Chief Investigator	No. of Users
	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 Chathanathodi	1
NIT Rourkela	Effects of swirl and rotation on turbulent pipe flow	Dr. Bikash Sahoo	1
Pandit Deendayal Upadhyaya Shekhawati University, Sikar	Ab initio Molecular Dynamics simulation of Ionic Liquid doped Polymer Electrolyte Membranes and Platinum Electrode Interface	Dr. Anurag Prakash Sunda	1
Panjab University	First principles study of hetero-structures of Phosphorene	Dr. Tankeshwar Kumar	2
Physics Department, Goa University	Study of Electronic, optical and thermodynamic properties of ABO ₂ type semiconductors	Dr. K R S Priolkar	2
PJTSAU, Hyderabad	Multi Omic Platform	Dr. M N V Prasad Gajula	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
SASTRA University	Hydrogen Storage on Alkali Metal Functionalized Porous Discrete Organic	Dr. Venkataramanan N S	2
	Inclusion Complexes of Cisplatin and its Analogues	Dr. A. Suvitha	1
SINP Kolkata	Structure, Dynamics and Interaction of Nuclear Acids	Prof. Dhananjay Bhattacharyya	2
SP Pune University	Computational studies of the aggregation of patchy particles under non-equilibrium conditions	Dr. Ahmed Sayeed	3

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Table A.1 – Continued from previous page

Institution	Project	Chief Investigator	No. of Users
	First-principles investigation of semiconductor nanostructures	Prof. Anjali Kshirsagar	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
	Effect of substitutional doping on electronic structure of II-VI semiconductor quantum dots	Prof. Anjali Kshirsagar	2
	Ab initio studies of doped GaNbO ₄ and TiO ₂ materials	Dr. Vaishali Shah	2
SRM University	Theoretical modeling of novel nanoelectronic devices	Dr. Arijit Sen	3
St. Xavier's College, Ahmedabad	Quantum transport in elemental doped boron nitride monolayer	Dr. Sanjeev Kumar Gupta	1

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Table A.1 – Continued from previous page

Institution	Project	Chief Investigator	No. of Users
University of Rajasthan, Jaipur	Observations of Gold Based Nanocatalysis at nanoscale	Dr. Devendra Kumar Mahawar	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

Total projects added in FY 2015-16 : 50

Appendix B

User's Experience with Dedicated Slot Booking Facility

" We have received comments from referees of Nucleic Acid Research (NAR) Journal asking us to re-perform the MD simulations using the latest force field parameters set and were given 60 days time to complete it. Without this dedicated slot it would have taken us a long time to complete the simulations we have performed during these two slots. We still need bit more computational time to finish some more simulations to prove our hypothesis. Considering the amount of computational time needed and time we have at our hand to submit the revised version, it would have been impossible to carry out these simulations on a regular queue. These two dedicated slots proved to be of tremendous important for revision of our manuscript submitted to NAR."

Mr. Sagar Khavnekar ,
Dr. Avinash Kale (Chief Investigator)
UM-DAE Centre for Excellence in Basic Sciences

" Nudge Elastic Band (NEB) calculations are expensive calculations and need to be run without any interruption in order to find the correct transition path. Other jobs which were expensive in terms of computational time were completed during this slot."

Mr. Subrhamanyams S.
Dr. Prasenjit Ghosh (Chief Investigator)
IISER Pune

" Both band structures and nudged elastic band calculations are expensive and require a relatively larger number of cores and memory. Although the converged path was not obtained for nudged elastic band calculations, there has been progress in the same direction."

Mr. Rohit Babar
Dr. Mukul Kabir (Chief Investigator)
IISER Pune

" This slot booking facility help me a lot. During this period as everyday a fix amount of nodes are fixed to me, so I can run all possible calculation in a systematic manner and get

a comparative study. In normal queue this work takes nearly a month.”

Mr. Debashish Das
Prof. Subhradip Ghosh (Chief Investigator)
IIT Guwahati

” In the off-stoichiometric compound of Mn_2NiSn/In , there are many functional properties around martensitic transformation. For better functionality of this material, it is very important to understand atomic ordering in different sub lattices and the electronic structure of these materials. During this slot, we have tried to explore the martensitic transformation with different sub lattice occupancy. The job runs faster than the job in regular queue.”

Mr. Ashis Kundu
Prof. Subhradip Ghosh (Chief Investigator)
IIT Guwahati

” Both band structures and nudged elastic band calculations are expensive and require a relatively larger number of cores and memory. Although the converged path was not obtained for nudged elastic band calculations, there has been progress in the same direction.”

Mr. Chandan Singh
Dr. Mukul Kabir (Chief Investigator)
IISER Pune

” Yes it is very useful , mainly for saving time and one can submit unlimited jobs (according to allocated cores).”

Mr. Yogeeshwar Ajjugal
Dr. Thenmalarchelvi Rathinavelan (Chief Investigator)
IIT Hyderabad

” Dedicated slot allowed me to keep a track of various computational experimentation needed, continuously. Long waiting times in the regular queue make it difficult to do so otherwise. We would like to request you to reduce the maximum walltime allowed for the regular queue. In the present scenario, the waiting period in the queue is huge enough to loose track of the submitted jobs. I would suggest that we should change the `max_wall_time` to 2/3 days and `max_running_jobs` 3 (and waiting 3) to keep the queue moving. Dedicated slots can be booked by those who can not continue a job after a break. Most of the VASP/QE/GROMACS/GAMESS users should be able to restart their jobs with little effort.”

Mr. Vaibhav Kaware
Dr. Kavita Joshi (Chief Investigator)
CSIR-NCL, Pune

” Current simulations are quite expensive with respect to computational cost. It is good to have some commands about how we are utilizing resources while running our jobs. The

bbcp command is very useful in this dedicated slot (since we have to transfer data to and fro effectively while using slot). I would like to thank personally for the continuous and constant help from npsfhelp@cdac.in. I would like to express my gratitude for extending disk space quota."

Mr. Subrahmanyams S.
Dr. Prasenjit Ghosh (Chief Investigator)
IISER Pune

" The molecular clusters we are contemplating are having countless possibilities. All potential possibilities need to be probed to make conclusive remarks. Thus, incessant availability of computational power to attempt each possibility imposes constraints on this path. However, with dedicated computer time for C-DAC state-of-art hardware, we have completed many sub-parts of computations."

Mr. Nityanand Sahu
Prof. Shridhar R Gadre (Chief Investigator)
IIT Kanpur

" Normally, The above mentioned task could have taken 1.5 months to complete."

Mr. Mandar Kulkarni
Dr. Arnab Mukherjee (Chief Investigator)
IISER Pune

" It helped me run few tests in quick time."

Mr. Sangkha Borah
Dr. Padma Kumar Padmanabhan (Chief Investigator)
IIT Guwahati

" We could use larger number of cores without being in a queue."

Ms. Deepashri Saraf
Dr. Anjali Kshirsagar (Chief Investigator)
Center for Modeling and Simulation, S. P. Pune University, Pune

" With the dedicated slot, we were able to simultaneously carry out more number of jobs without any waiting period."

Ms. Sanjana Nair, Mr. Venkata Subbaiah SP
Dr. Thenmalarchelvi Rathinavelan (Chief Investigator)
IIT Hyderabad

"The job in dedicated slot queue run a bit faster than regular job queue. The results that we have got using dedicated slot queues, would have taken 6-7 month in regular job queues."

Mr. Ashis Kundu, Mr. Srikrishna Ghosh
Prof. Subhradip Ghosh (Chief Investigator)
IIT Guwahati

" Nudge Elastic Band (NEB) calculations are expensive calculations and need to be run without any interruption and difficult to converge in order to find the correct transition path."

Mr. Nandha Kumar
Dr. Prasenjit Ghosh (Chief Investigator)
IISER Pune

Some appreciation messages from user's

"As my students who are accessing PARAM Yuva gave me a positive feed back on the computing resources, I have requested my new PhD students as well to get an account."

Dr. Gopalan Rajaraman
Associate Professor
IIT Bombay

"I remain highly thankful to C-DAC, Pune for the National PARAM Supercomputing Facility (NPSF) provided to my research group on PARAM-Yuva II."

Dr. Abir De Sarkar
Associate Professor
INST, Mohali

"I heartily wish your entire team, a very happy, prosperous and successful new year. 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
Assistant Professor
Amity University

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

"Thank you for providing such a wonderful support and a world class facility!"

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

Appendix C

Picture Gallery



Dr. Sandeep Joshi delivering talk on *Parallel Computing* at IISER, Mohali workshop



Dr. Venkatesh Shenoi delivering talk on *Optimization of PDE Solvers* at IISER, Mohali workshop



Mr. Pankaj Dorlikar delivering talk on *Leveraging multicore with OpenMP* at IISER, Mohali workshop



Ms. Chaitali Chandratre delivering talk on *Going beyond multicore : HPC using message passing* at IISER, Mohali workshop



Ms. Nisha Agrawal delivering talk on *Performance considerations and uniprocessor optimization techniques* at IISER, Mohali workshop



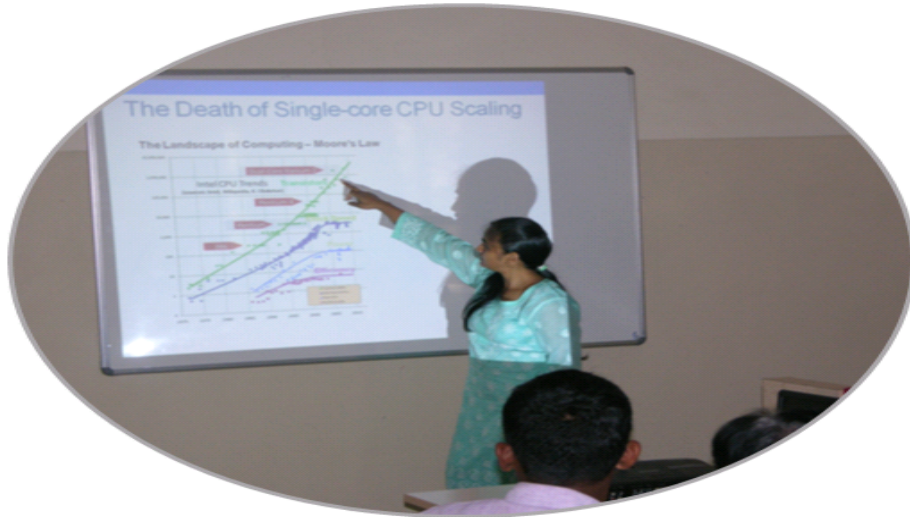
NPSF team members during IISER, Mohali workshop



Mr. Pankaj Dorliker delivering invited talk on *Computer Architecture for Scientific Computing* at S. P. Pune Univ.



Mr. Y. S. Swarup delivering invited talk on *HPC Technologies & Job opportunities* at SKBR college, Amlapuram



Ms. Nisha Agrawal delivering invited talk on *Introduction to OpenCL Computing* at PICT, Pune



Mr. Y. S. Swarup, explaining about NPSF on National Science Day, C-DAC, Pune



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



Mr. Gaurav Kumar Marskole, explaining about NPSF on National Science
Day, C-DAC, Pune



Mr. Maneesh Kumar, explaining about NPSF on National Science Day,
C-DAC, Pune



Mr. Arun Gupta, 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

PARAM Series of Supercomputers



PARAM Yuva II