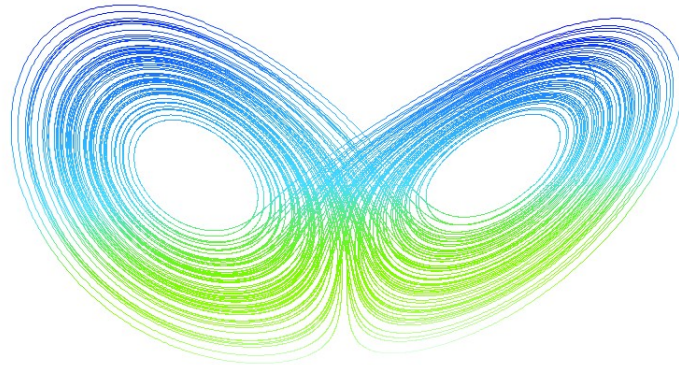


Annual Report
of
National PARAM Supercomputing Facility



2013-14



Centre for Development of Advanced Computing, Pune

Message From Director General, C-DAC

Computational Science has emerged as an active area of research in various branches of Science and Engineering. The scenario in India is quite encouraging, with the involvement of good number of researchers in the area of HPC applications, in keeping up with the global trend.

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

The upgrade of PARAM Yuva to PARAM YuvaII has helped C-DAC to join the Petascale league of Supercomputing centres. C-DAC in general and NPSF in particular had a remarkable year in 2013 with PARAM YuvaII achieving coveted ranks in both Top500 and Green500 lists. The efficient maintenance and management of the facility, promotion of users and the user support have been among the primary mandates of NPSF.

This report summarizes the activities of NPSF during the year 2013-2014 and showcases the science pursued by the Indian scientific community using this facility. I appreciate the efforts of NPSF group for their contributions to nation's HPC programme. I look forward to their continued commitment in managing a world class computing facility at C-DAC for the researchers in the years to come.



Prof. Rajat Moona
Director General, C-DAC

Message From Executive Director, C-DAC, Pune

The start of 2013 was marked with big changes to the National PARAM Supercomputing Facility (NPSF). NPSF now has more than 10 talented and dedicated staff, and continues to grow. The activities of NPSF include training, collaboration, and events conducted for the public apart from the usual support activities. Combined with our data-center NPSF will continue to have the best facilities of any advanced computing center, and lots of room for growth in our team and our systems.



The present space, power & cooling infrastructure has been put to good use with the launch of PARAM Yuva II at the start of this year. PARAM Yuva II augments PARAM Yuva as our premier computing resource. Unlike PARAM Yuva, PARAM Yuva II is equipped with the Intel Xeon Phi and Nvidia GPUs. Unlike any system we have had in the past, we will be keeping part of PARAM Yuva II available for *interactive* use, allowing scientists and engineers to explore their data sets in real time through visualization and other exploration tools. PARAM Yuva II is supported by a large high performance storage to push NPSF forward into data intensive computing.

And while all this is happening, PARAM Yuva II just had its first birthday and still has few great years ahead. In its first year of operations, PARAM Yuva II exceeded our expectations; around 134 different science and engineering research projects took advantage of the system to run around 80,000 jobs on the system, with about 500 researchers running jobs. All of these numbers continue to climb, as PARAM Yuva II proves to be an invaluable productive instrument for the Indian scientific community.

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

Message From Senior Director, C-DAC

As I pen this message, I recall the day when C-DAC's National PARAM Supercomputing Facility (NPSF) was established in March 1998 along with the launch of PARAM 10000 system built by C-DAC. I was entrusted with the task of managing this unique facility of the nation. The mandate of NPSF was to offer state-of-the-art High Performance Computing (HPC) systems to the HPC user community, help them with the know-how and usage of such systems, and proliferate HPC-awareness in the country.

We immediately defined a Technical Affiliation Scheme for NPSF, detailing its various services, entry and eligibility criteria for NPSF Technical Affiliates (users), charging policies, remote access mechanisms, and security policies and mechanisms. We also detailed the processes for round-the-clock operations of the facility and commissioned a group of system administrators, parallel programming experts, and maintenance staff to offer supercomputing services to the HPC users. All these initiatives contributed to the proliferation of parallel and distribute processing technologies in India and helped several researchers from various scientific and engineering disciplines to carry out their research more effectively.

We at C-DAC have always ensured that NPSF offers world-class HPC systems and services to its affiliates. To meet this objective, NPSF team upgraded its system's capability this year to make it the first system in the country (PARAM Yuva II) to cross the half PetaFlop peak computing performance. While the compute power of PARAM Yuva II is ten times that of its predecessor system, its power consumption remains the same. Hence, the system has enabled us to provision far better computing capability to the HPC user community of the country at similar operational cost as before.

Today, I feel satisfied that over the years, NPSF group has matured into running a world-class supercomputing facility. The group's efforts have helped in building the culture in Indian scientific and research community of using the most powerful R&D tool today (the supercomputers) for carrying out cutting-edge R&D and problem solving in various domains of science and engineering. The user base of the supercomputing systems in the country has increased many-fold today as compared to the days when NPSF was first established in the country. A fair share for this positive movement can certainly be attributed to the NPSF of C-DAC.



Dr. Pradeep K. Sinha
Senior Director,
Corporate Strategy and R&D, C-DAC

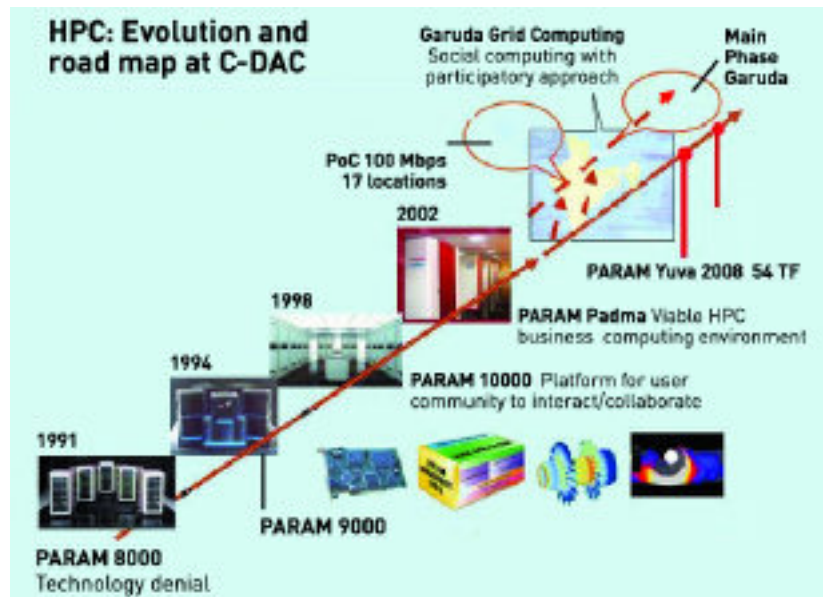
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1

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 68th 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 YuvaI, 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 / coprocessor 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 has also set up a National PARAM Supercomputing Facility (NPSF) at C-DAC, Pune to facilitate the access of HPC resources required to solve compute-intensive problems of researchers around the country. 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. Please refer to NPSF portal <https://yuva.cdac.in/> for details.

This report documents the activities of NPSF undertaken during the year 2013.

2

Projects 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 through the following three major projects over the recent past years. The projects are listed below with brief details of their deliverables / milestones.

1. National PARAM Supercomputing Facility and Next Generation HPC technologies (DIT/R&D/C-DAC/2(2)/2008, dt. 25/05/2008)

[Duration: 26/05/2008 - 26/05/2011, Status: Completed]

Focus:

- Site preparation activities, including site layout, power sizing, cooling setup, and placement of system stacks
- System integration of components and sub-components including computing, networking, storage, and other resources into a unified supercomputing system (PARAM Yuva I)
- Proper configuration of the system to ease its usage as a cluster, including integration with the batch processing system
- Installation and integration of the three tier storage with the system
- Development of a web application for secure remote access of the system for users (PARAM Yuva portal)
- Development/customization and installation of required tools for monitoring and management of smooth operations of PARAM Yuva I facility
- Porting scientific applications across various domains
- Operate NPSF and support users of PARAM Yuva I
- Integration of PARAM Yuva I with India's national computing grid GARUDA
- Enable users of PARAM Yuva I through NPSF Technical affiliate scheme

2. Power Optimization of HPC System and Facility (DIT/R&D/C-DAC/2(7)/2010, dt. 28/03/2011)

[Duration: 01/04/2011 - 31/03/2013, Status: Completed]

Focus:

- Development of policy engine for enabling switching from high power to low power/idle state

- Implementation of power aware scheduler on the production system (PARAM YuvaI)
- Incorporation of ‘power’ state in monitoring tools (Ganglia & Xymon)
- Feedback driven policy engine & power policy implementation

3. 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 - 31/03/2014, Status: Ongoing]

Focus:

- Upgrade of PARAM YuvaI 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

2013

January

Upgrade of the facility, testing and completion of the first benchmarking exercise on Jan. 30.



Rearrangements in progress to pave the way for PARAM Yuva II.



Assembly of new systems.

February

Workshop on **National Supercomputing Mission** was organized on Feb. 8, which was

attended by delegates from Institutes, National Labs, NITs, IITs, and Universities, to deliberate on the future of HPC in India. The launch of PARAM Yuva II coincided with the workshop.

Dedicated PARAM Yuva II to the Indian scientific community on February 20, 2013.

March

Promotion of new users and installation of applications.

April

Two day **Intel Xeon Phi Training** was conducted by Intel expert team constituting, Dr. Sunil Sherlekar, Dr. Pradeep Dubey, Mr. Dhiraj Kalamkar, Mr. Rama Malladi, Mr. Naveen Mellempudi Dr. Ganesh Bikshandi and Mr. Jaiber John on Apr. 29 & 30. This was attended by members of the HPC groups of C-DAC. Some of the NPSF users joined the training session through Google hangout.

May

Visit by Prof. Mahendra K. Verma and his students from IIT, Kanpur for the scaling exercise of the home grown CFD code TARANG on PARAM Yuva II. Prof. Verma delivered a talk, titled “Porting of spectral simulator TARANG to PARAM Yuva II”, sharing the experience at the end of two week long exercise on May 24.

Benchmarking exercise for Top500 ranking: May 27-30. PARAM Yuva II with sustained performance of 386.7 TFlops was ranked 69th in the June 2013 Top500 list.

July

Five member team from NPSF constituting Ms. Chaitali Chandratre, Ms. Nisha Agarwal, Mr. Rishi Pathak, Dr. Sandeep K. Joshi, and Dr. V. Venkatesh Shenoi conducted a day long session on July 1, covering various aspects of High Performance Computing as part of **Faculty Development Programme** (July 1-5) at Walchand College of Engineering, Sangli.

August

Mr. Y. S. Swarup and Dr. Sandeep K. Joshi visited INS Valsura, Jamnagar as part of technology update programme. Dr. Joshi delivered a lecture on “Supercomputing”.



Dr. Joshi's lecture at INS, Valsura.

September

Half a day workshop was conducted on (23/09) by Dr. Werner Krotz-Vogel from Intel, covering “Intel road map on future architecture” and “Intel Xeon Phi: Architecture,

Programming Models and Optimization”.

Prof. Bhanu P. Das, IIA, Bangalore visited C-DAC between Sept. 22-25 for interactions with HPC groups.

October

Dr. Bobby Phillip, Senior Scientist, ORNL (USA) visited C-DAC on Oct. 15 for interactions with the HPC groups to identify areas of collaborations between C-DAC and ORNL.



Dr. Phillip visiting the computing facility.

Benchmarking exercise for Green500 ranking: Oct. 28 - Nov 5. PARAM Yuva II with performance of 1,760.20 MFlops per Watt was ranked 44th in the November 2013 Green500 list.

November

Workshop on **Application Optimization on Intel Xeon Phi** was conducted by Intel between Nov. 25-30. The Intel expert team of Dr. Arvind Amin, Dr. Christopher Dahnken, Mr. Indraneil Gokhale, and Ms. Sudha Thiagarajan interacted with different groups and mentored the activities.

December

The Intel intervention on optimization continued for the second week between Dec. 2-7.

2014

January

Visit by Intel expert Dr. Arvind Amin (11/01 & 13/01) for interactions with application groups of C-DAC, on optimizing applications on Intel Xeon and Xeon Phi.

February

NPSF annual review meeting to review NPSF activities by C-DAC senior management was conducted on Feb. 15, 2014

Dr. Sandeep K. Joshi gave an invited talk titled “Power and Energy Consumption Optimization in HPC Facilities: An Overview” on Feb. 21, in the **National Conference on**

Energy and Environment organized by University of Pune.

Students from Colleges and schools visited NPSF during C-DAC Science Day celebrations on Feb. 28.

March

Computing resources support for HPC workshop at IIT, Delhi and HPC competition as part of Techkriti '14 at IIT, Kanpur.

4

PARAM Yuva II Milestones

Inauguration



PARAM Yuva II was inaugurated by Shri. J. Satyanarayana, Honourable Secretary, DeitY, Government of India on February 8, 2013 at National PARAM Supercomputing Facility in the C-DAC premises on the Pune university campus. PARAM Yuva II with theoretical peak performance of 529.4 Tera Flops is about 10 times faster than PARAM Yuva I.

PARAM Yuva II with a sustained performance of 386.7 Tera Flops was ranked 69th in the TOP500 list of supercomputers released in June 2013 at the International Supercomputing Conference '13 at Leipzig, Germany. PARAM Yuva II relies on Intel Xeon Phi for its computing power, thus making it energy efficient than its predecessor thus boosting the Flops per Watt index. PARAM Yuva II with the performance of 1,760.20 MFlops per Watt was ranked 44th in the "Green500" list released in November 2013 at the Supercomputing conference '13 at Denver, Colorado, USA. The present rank of the system as per the November 2013 TOP500 list is 83.

Top500 Ranking <http://www.top500.org>



Green500 Ranking <http://www.green500.org>



5

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

- 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
- 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
- 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
 - Two NVIDIA GPU Tesla M2090 per node

Storage:

- HPC Scratch area with 10 GB/s write bandwidth over Parallel File System
- Reliable User Home Area: 100TB
- Backup: 400TB (native capacity)

Software:

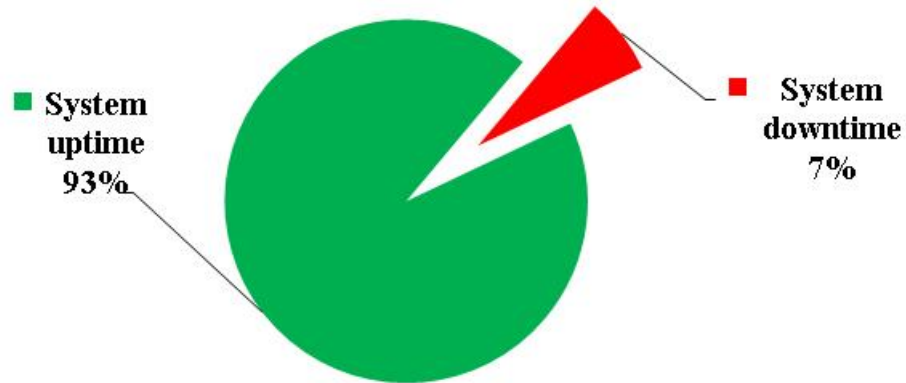
- Operating System: Cent OS v6.2, Kernel v2.6.32-220
- Intel Cluster Studio XE 2013
- PGI Cluster Development Kit

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

Resource Availability: (Period: Jan. 1, 2013 - Mar. 31, 2014) [455 Days]

PARAM Yuva II system availability



- Uptime: \approx 423 Days
- Maintenance Period: \approx 32 Days
 - Mar. 30, 2013, 09:00 AM - Apr. 01, 2013, 11:00 AM [3 Days, 2 Hrs]
 - Jun. 01, 2013, 10:00 AM - Jun. 07, 2013, 11:00 AM [7 Days, 1 Hr]
 - Oct. 02, 2013, 10:00 AM - Oct. 03, 2013, 11:00 AM [25 Hrs]
 - Dec. 13, 2013, 10:00 AM - Dec. 24, 2013, 04:00 AM [11 Days, 6 Hrs]
 - Jan. 27, 2014, 10:00 AM - Feb. 01, 2014, 06:00 PM [5 Days, 8 Hrs]
 - Mar. 25, 2014, 10:00 AM - Mar. 28, 2014, 08:00 PM [3 Days, 10 Hrs]
- TARANG (CFD code) Scaling exercise
 - May 12, 2013 - May 26, 2013 [15 Days]
- Benchmarking:
 - May 27, 2013, 10:00 AM - Jun 01, 2013, 10:00 AM [Top500 Ranking]
 - Oct. 28, 2013, 2:00 PM - Nov. 05, 2013, 3:00 PM [Green500 Ranking]

6

Projects, Users & Usage Statistics

Projects & Users (as of 31st March 2014)

- Number of projects : 134
- Number of users: 596 (across 41 Institutions)

Users across Institutions

Table 6.1: Users across Institutions

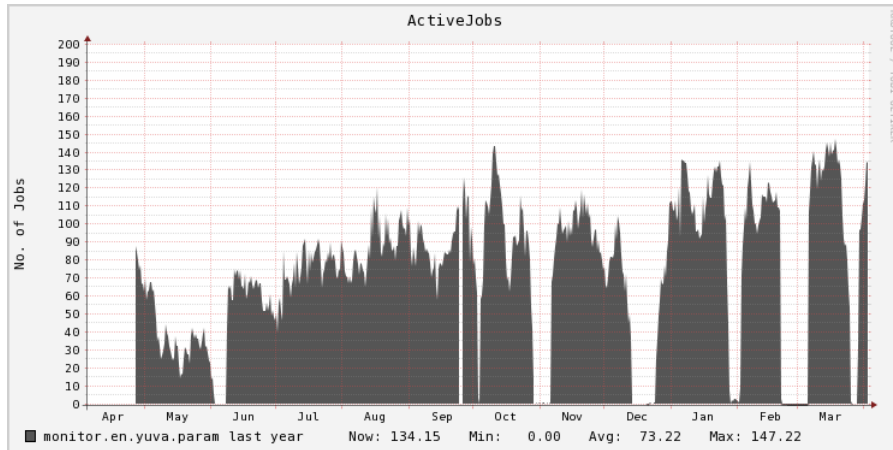
Institution	No. of Users
Ahmednagar College	1
Amity University	1
Anna University	2
BARC, Mumbai	1
CMR College of Eng. & Tech	2
Carnegie Mellon University	1
C-DAC	100
CECRI, Karaikudi	1
GARUDA	165
Gunanak Dev University	1
Himachal Pradesh Univesity	3
IASST, Guwahati	3
IIA, Bangalore	8
IISC, Bangalore	5
IISER, Pune	23
IIT Bombay	121
IIT Delhi	38
IIT Guwahati	12
IIT Gandhinagar	4
IIT Hyderabad	6
IIT Jodhpur	2
IIT Kanpur	18
IIT Kharagpur	6
IIT Ropar	8
ISRO	5

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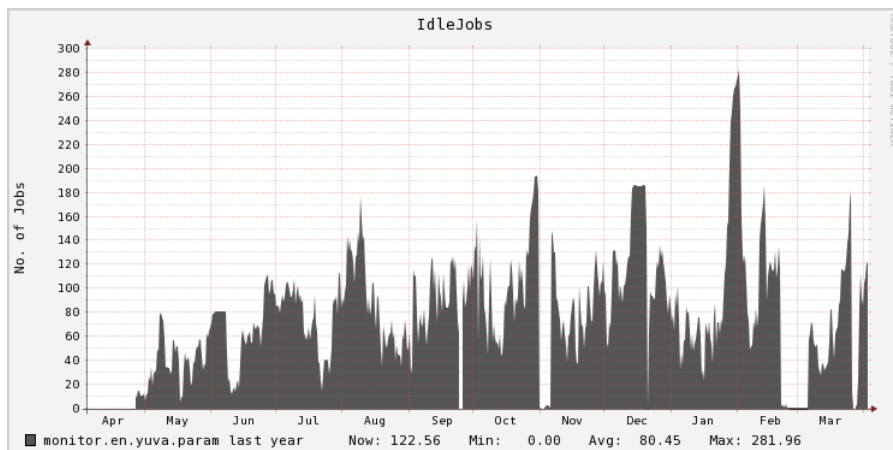
Table 6.1 – Continued from previous page

Institution	No. of Users
IUCAA, Pune	5
Jiwaji University	3
JNCASR, Bangalore	3
JNU	2
MIT, Pune	1
NABI, Mohali	1
NCL, Pune	2
NCRA, Pune	6
NIC	2
NIT Calicut	1
PRL, Ahmedabad	3
RRI, Bangalore	3
RTM Nagpur University	2
SRM University	3
University of Pune	16
Vijay Kumar Foundation, Gugaon	5
VNIT Nagpur	1
Total	596

Job Queues: Running Jobs (Active Jobs)

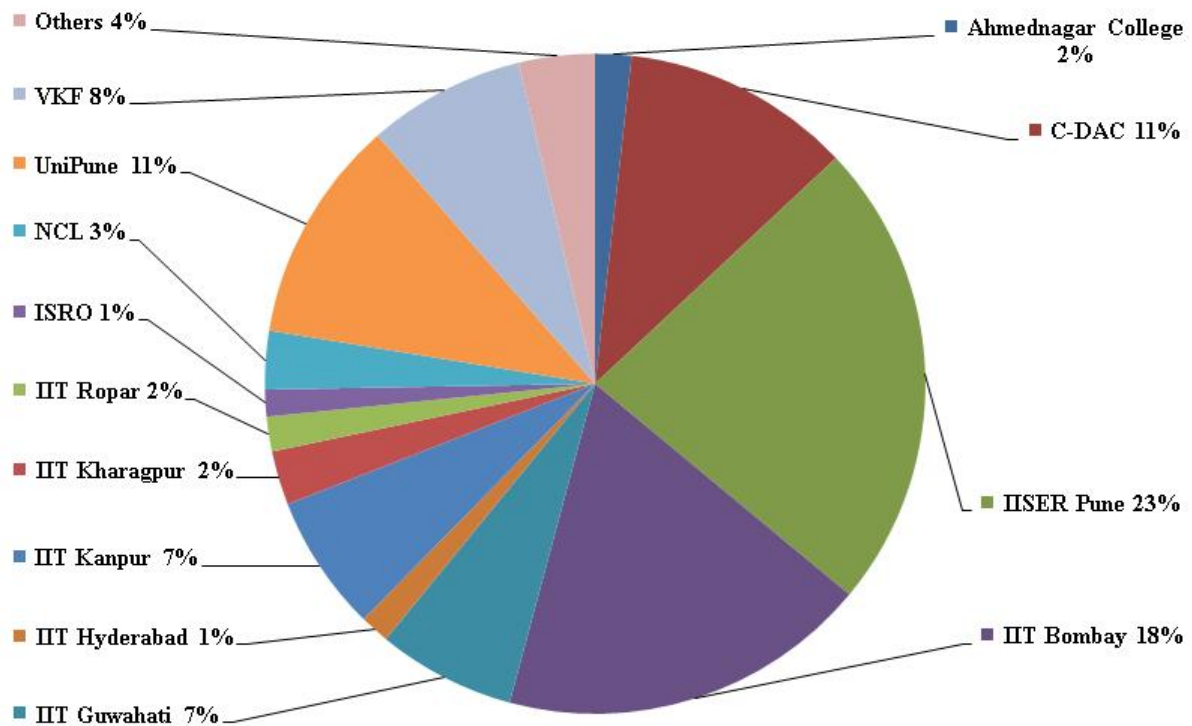


Job Queues: Idle Jobs - Jobs waiting in queue to start running

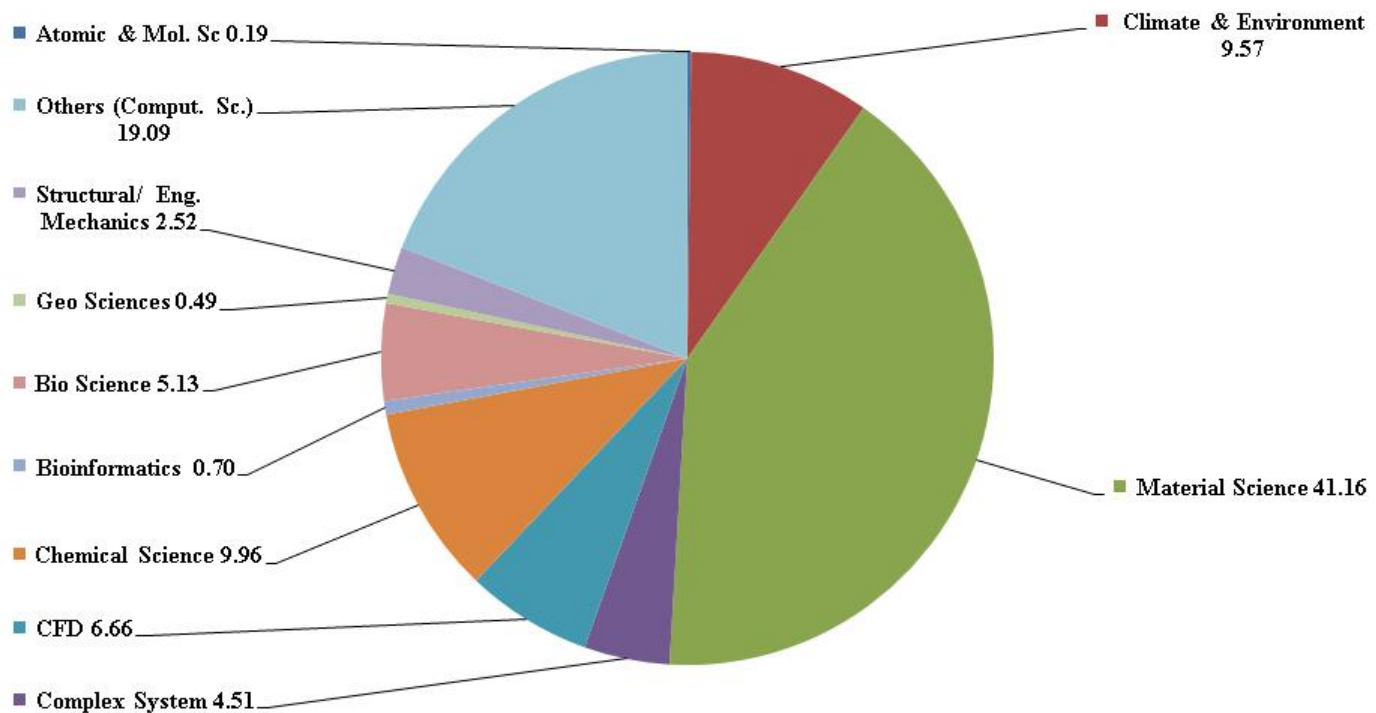


CPU Utilization

Institute wise CPU utilization (in %)

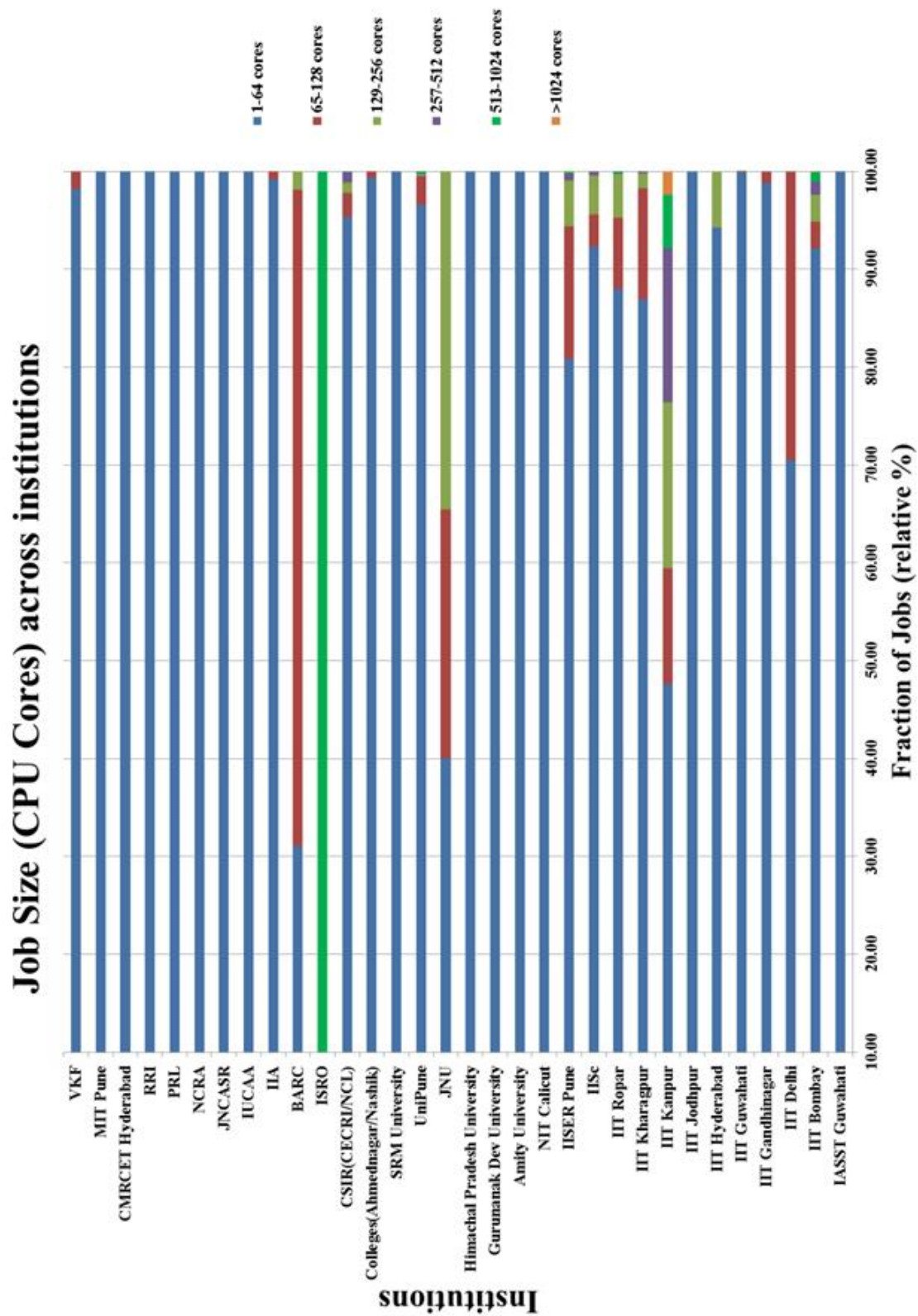


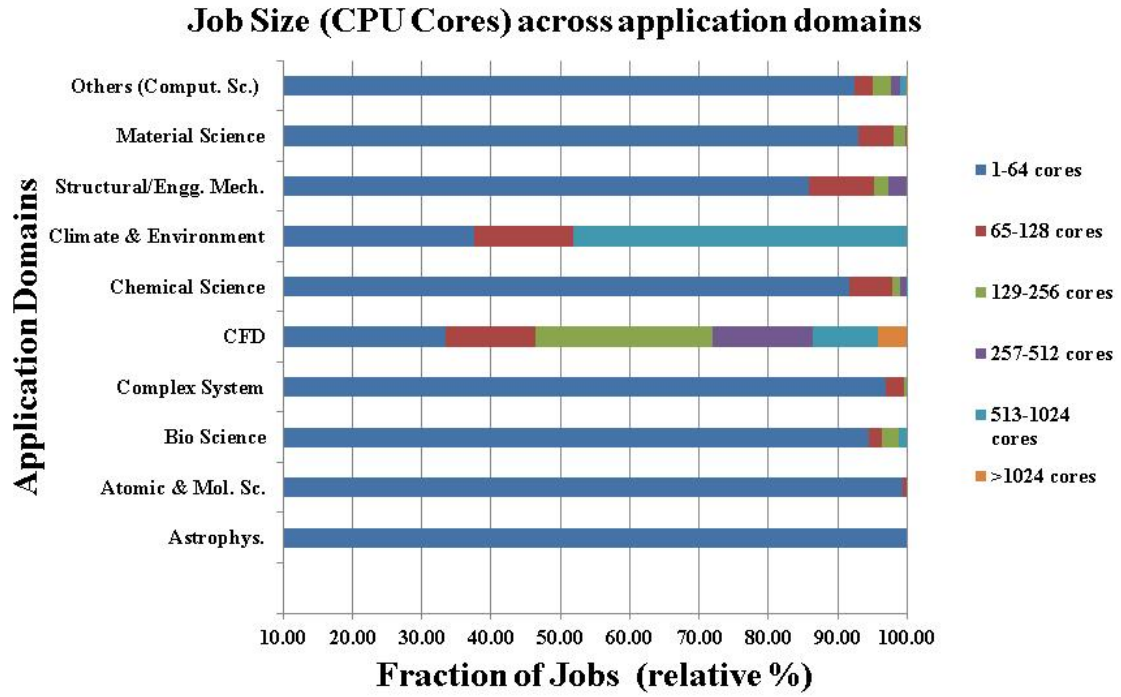
CPU time utilization (in %) across application domains



Job Statistics

External Users:





All Users:

Total Number of Jobs= 87136 (Period: Jan. 1, 2013 - Mar. 31, 2014)

Jobs across Domains

Table 6.2: Jobs across Domains

Domain	Jobs
Astrophysics	99
Atomic & Mol. Sc	166
Bioinformatics	420
Bio Science	1549
CFD	3253
Climate & Environment	13682
Complex System	2255
Chemical Science	6762
Geo Sciences	1137
Material Science	36512
Structural/ Eng. Mechanics	3288
Others (Comput. Sc.)	18013
Total	87136

7

Major Research Projects

Investigation of semiconducting nanoclusters using first principle calculations

Dr. Pradip Shelke, Ahmednagar College, Ahmednagar

Structure and dynamics of deposited metal clusters

Dr. Chiranjib Majumder, BARC, Mumbai

To study the atomic and electronic structure of III-V semiconductor nanostructures

Prof. S. S. Sekhon, Gurunanak Dev University, Amritsar

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

Structural deformations of DNA and relation to intercalation mechanism

Dr. Arnab Mukherjee, IISER, Pune

Molecular modelling and dynamics of polymers, gas hydrates and ionic liquids: An alternative energy initiative

Dr. Arun Venkatnathan, IISER, Pune

Study of CdS and CdTeS quantum dots decorated on TiO₂ nanowires

Dr. Prasenjit Ghosh, IISER, Pune

High Performance Computing initiative (IIT, Bombay)

Prof. Alok Shukla (Material Science), Dr. Ganesh A. Viswanathan (Bio Science)

Electronic structure and dynamics

Dr. Aditya N. Panda, IIT, Guwahati

Shape and size effects of nanoparticles on the properties of polymer nanocomposites

Prof. Jayant K. Singh, IIT, Kanpur

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

Study of complex fluid flows past bluff bodies
Prof. Sanjay Mittal, IIT, Kanpur

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

Open Source Drug Discovery (GARUDA)
Dr. Vinod Scaria, IGIB, New Delhi

Investigation of finite temperature behaviour of finite size systems
Dr. Kavita Joshi, NCL, Pune

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

First-principles investigation of semiconductor nanostructures
Prof. Anjali Kshirsagar, University of Pune

Investigation of structural and optical properties of semiconducting materials in various forms
Prof. S. V. Ghaisas, University of Pune

Ab initio studies of materials: nanostructures, defects, surfaces and bulk metallic glasses
Prof. Vijay Kumar, Dr. Vijay Kumar Foundation, Gurgaon

8

Science using PARAM Yuva II

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.

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

Advanced Materials (14.829)

Pradip B. Shelke, D. Nguyen, A. V. Limaye, and P. Schall, Controlling colloidal morphologies by critical Casimir forces, *Advanced Materials* **25**, 1499 (2013).

Physical Review Letters (7.943)

M. Chandra and M. K. Verma, Flow Reversals in Turbulent Convection via Vortex Reconnections, *Phys. Rev. Lett* **110**, 114503 (2013).

Journal of Physical Chemistry Letters (6.585)

I. Kaul, N. Joshi, N. Ballav, and P. Ghosh, Hydrogenation of Ferrimagnetic Graphene on a Co Surface: Significant Enhancement of Spin Moments by C-H Functionality, *J. Phys. Chem. Lett.* **3**, 2852 (2012).

J. P. Furtado, A. P. Rahalkar, S. Shanker, P. Bandyopadhyay, and S. R. Gadre, Facilitating Minima Search for Large Water Clusters at MP2 Level via Molecular Tailoring, *J. Phys. Chem. Lett.* **3**, 2253 (2012).

ACS Catalysis (5.265)

S. Santra, P. K. Hota, R. Bhattacharyya, P. Bera, P. Ghosh, and S. K. Mandal, Palladium Nanoparticles on Graphite Oxide: A Recyclable Catalyst for the Synthesis of Biaryl Cores, *ACS Catalysis* **3**, 2776 (2013).

Journal of Physical Chemistry C (4.814)

D. Bhandary, S. Khan, and J. K. Singh, Structure and Dynamics of n-Alkanol Monolayers on a Mica Surface, *J. Phys. Chem. C* (2014). (*Accepted*)

P. P. Ingole, G. B. Markad, D. Saraf, L. Tatikondewar, O. Nene, A. Kshirsagar, and S. K. Haram, Band Gap Bowing at Nanoscale: Investigation of $\text{CdS}_x\text{Se}_{1-x}$ Alloy Quantum Dots through Cyclic Voltammetry and Density Functional Theory, *J. Phys. Chem. C* **117**, 7376 (2013).

A. B. Rahane, M. D. Deshpande, and V. Kumar, First Principles Calculations for Structural, Electronic, and Magnetic Properties of Gadolinium-Doped Alumina Clusters, *J. Phys. Chem. C* **116**, 6115 (2012).

A. B. Rahane and M. D. Deshpande, Structural and Electronic Properties of Neutral and Ionic $(\text{Ga}_2\text{O}_3)_n$ Clusters with $n = 1-10$, *J. Phys. Chem. C* **116**, 2691 (2012).

Crystal Growth & Design (4.689)

S. A. Acharya, N. Maheshwari, L. Tatikondewar, A. Kshirsagar and S. K. Kulkarni, Ethylenediamine-Mediated Wurtzite Phase Formation in ZnS, *Crystal Growth & Design* **13**, 1369 (2013).

Journal of Physical Chemistry B (4.189)

A. P. Sunda, V. M. Dhavale, S. Kurungot, and Arun Venkatnathan, Structure and Dynamics of Benzyl-NX3 ($X = \text{Me}, \text{Et}$) Trifluoromethanesulfonate Ionic Liquids, *J. Phys. Chem. B* (2014). (*Accepted*)

Soft Matter (3.91)

T. K. Patra and J. K. Singh, Polymer directed aggregation and dispersion of anisotropic nanoparticles, *Soft Matter* (2014). (*Accepted*)

Physical Chemistry Chemical Physics (3.829)

H. Sahu and A. N. Panda, Computational investigation of charge injection and transport properties of a series of thiophene-pyrrole based oligo-azomethines, *Phys. Chem. Chem. Phys.* (2014). (*Accepted*)

A. Kshirsagar and D. Saraf, Electronic structure at nanocontacts of surface passivated CdSe nanorods with gold clusters, *Phys. Chem. Chem. Phys.* (2014). (*Accepted*)

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European Physical Journal D (1.513)

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Silicon (1.417)

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Computational and Theoretical Chemistry (1.371)

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Journal of Chemical Sciences (1.298)

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M. K. Verma, A. Chatterjee, S. Paul, K. S. Reddy, R. Yadav, M. Chandra, and R. Samtanay, Benchmarking and scaling studies of a pseudospectral code Tarang for turbulence simulations, Pramana **81**, 617 (2013).

Publications by NPSF users (Both PARAM Yuva I & Yuva II)

- 2009 : 16
- 2010 : 17
- 2011 : 14
- 2012 : 22
- 2013 : 38 (including ones accepted for publication)

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PARAM Yuva II Visits

Visits by Officials, Members of Academia & Industry

1. Shri J . Satyanarayana, Honourable Secretary, DeitY and Dr.G.V.Ramaraju, Group Coordinator, R&D in IT, DeitY (Feb. 8, 2013).
2. Dr. Stephen Wheat, GM, Intel HPC Unit and Dr. Avinash Palaniswamy, Lead Member HPC group, Intel (Feb. 27, 2013).
3. Maj. Gen. R. J. Noronha, AVSM, SM (Mar. 5, 2013).
4. Prof. N. V. Deshpande, Director, NIT, Silchar (May 24, 2013).
5. Shri J. B. Mohapatra, Joint Secretary & Financial Adviser, DeitY (Aug. 21, 2013).
6. Shri Milind Deora, Honorable Minister of State for Communication and Information Technology (Oct. 25, 2013).
7. Mrs. Aruna Sundararajan, Managing Director, Kerala State Industrial Development Corporation (Feb. 2014).

Visits as part of various programmes

1. Participants (30) of the **Annual Monsoon-2012 Workshop** organized by Indian Meteorological Society Pune Chapter, Feb. 19-20, 2013 (Feb. 19, 2013).
2. Participants (28) of **Refresher Course for Teachers** organized by Department of Education and Extension, University of Pune (Nov. 29, 2013).
3. Officers from Indian Army, Brig. B. D. Rai, Brig. S. K. Narain, and Col. L. S. Lidder as part of **Bharat Dharshan Tour** by DAs/MAs(Designate) (Jan. 31, 2014).



Presentation to the students of Sinhagad College of Engineering on Sep. 12, 2013.

Industrial Visits for students

Institution	No.of visitors	Visit Date
2013		
Government College of Engineering, Avasari	63	Mar. 06
Nath Valley School, Aurangabad	55	Mar. 14
S. V. B. I. T., Gandhinagar	44	Aug. 30
Sinhagad College of Engineering, Pune	83	Sep. 12
St. Xavier's College, Ranchi	44	Oct. 20
2014		
Engineering college, Bangalore	50	Jan. 27
Saboo Siddik College of Polytechnic, Mumbai	43	Feb. 01

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Picture Gallery



Delegates present during the inauguration of PARAM Yuva II on Feb. 8 2013.



NPSF Annual Review meeting on Feb. 15 2014.



C-DAC Science Day Celebrations, Feb. 28, 2014: NPSF stall.



C-DAC Science Day Celebrations, Feb. 28, 2014: NPSF stall (contd.).

PARAM Series of Supercomputers



PARAM Yuva II