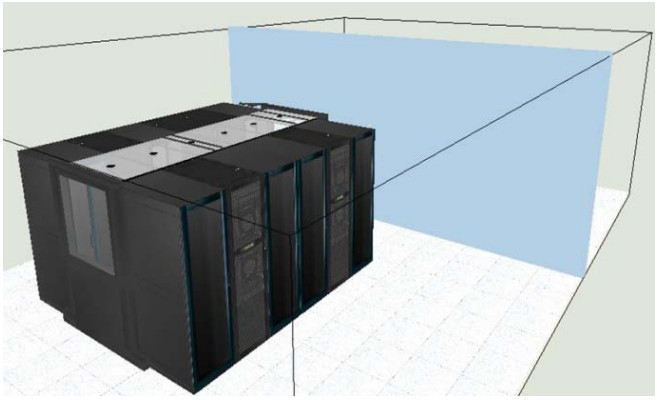
A Successful Journey: Vikram-100
High Performance Computing (HPC) Cluster of PRL
(June 2015-June2020)



Prepared By
Computational Services Group
High Performance Computing Committee

Physical Research Laboratory

Document Number	Issue Number	Month / Year	Classification	Control Status
PRL/HPC/Vikram100/062020	01	06/2020	General	Controlled
Copy Number	**Type**		**Number of Pages**	
01	Report		14	
Title: A Successful Journey: Vikam-100 High Performance Computing (HPC) Cluster of PRL				

Abstract	This document covers in brief the journey of Vikram-100, the 100 Teraflops (TF) High Performance Computing (HPC) Cluster facility at PRL.
Authors	Computational Service Group and High Performance Computing Committee
Reviewed & Approved By	Dr. Angom Dilip Kumar Singh, Chairman, High Performance Computing Committee
Submitted To	Director, PRL
Keywords	High Performance Computing, Cluster

Table of Contents

1. Introduction

Over the years, there has been a dramatic increase in the computing power and capabilities. The recent advances in Very Large Scale Integration (VLSI) technology have played a major role in the development of powerful parallel computers. There is also rapid progress in the software technology. Various software, like Operating Systems, Compilers, Programming Languages, and Tools are now available. This has enabled the development and deployment of sophisticated applications catering to the scientific research and engineering needs. The key reason for using parallel computers is that parallelism is one of the best ways to overcome the speed bottleneck of a single processor.

High Performance Computing (HPC) uses supercomputers and computer clusters to solve advanced computational problems. The term HPC has become very common in the modern scientific and engineering research. Today, computer systems in the teraflops/petaflops-region are considered as HPC systems.

2. Background

PRL had procured IBM RS6000/SP to cater the high-end computational requirements of the PRL scientific and technical faculties. It was operational during the period of 2002-2006. And, PRL scientific and technical faculty members used it heavily to run their various scientific applications and models. Around 2004 onwards, the era was to migrate and use open source technologies as it offered several benefits. PRL users also picked up this trend and started to migrate their applications on open source technology. At that time to meet the computational needs, the Computer Centre was equipped with four HP servers with 4GB RAM and 1.5TB storage and One Dell Server with 16CPU and 64GB RAM having Open Source Linux Operating System. Apart from this, Computer Centre had migrated all the services like File, Email, Web, Proxy completely on open source platform. The available computing resources were efficiently used to run various scientific applications and models build on open source technologies. However, better and faster computing power was needed to solve scientific problems proposed by PRL scientists and technical faculties as part of new scientific projects and programs. Apart from this, the computing resources were running on proprietary IBM AIX operating system, IBM Fortran, C and C++ compilers. So a need for system with scalable hardware, open source software like compilers, libraries was felt.

To cater this high end computational need, 2TF High Performance Computing (HPC) cluster was made available to the PRL users on November 27, 2009 and was operational till June 2015 i.e. till all the HPC users data migrated to the new 100TF HPC[3]. The entire system was setup using open source technologies like Red Hat Linux Operating System, ROCKS cluster suite and Ganglia cluster monitoring suite. This system had 20 Compute Nodes, 1 Master Node with 3TF peak and 2.2TF sustained computing performance.

The following four applications were migrated on new HPC cluster and users achieved significant performance improvement.

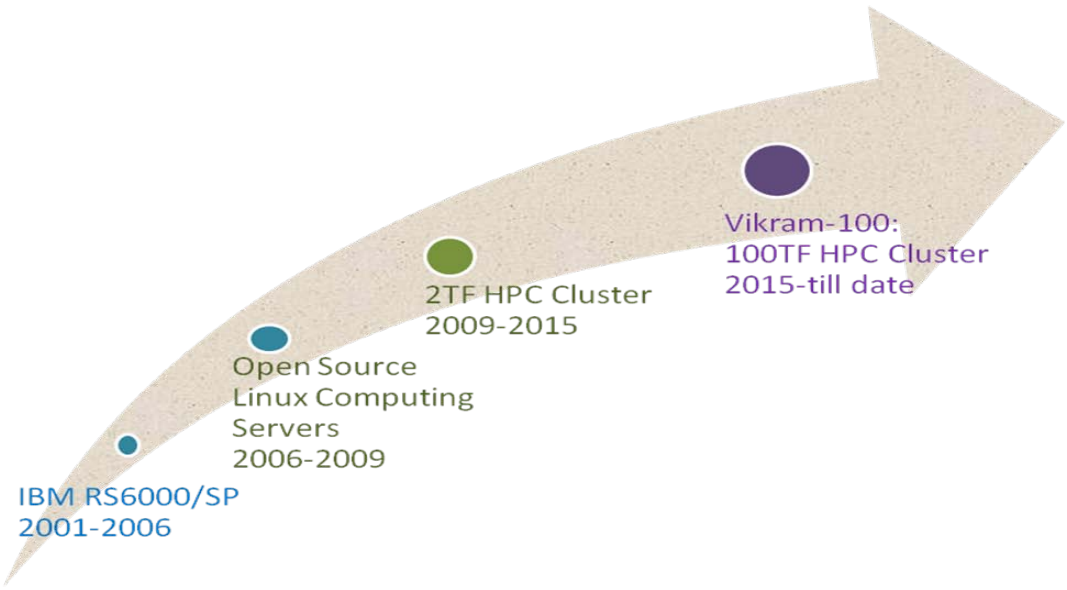
(a) Global Modeling of Atmospheric Ozone and Trace Gases in the Troposphere with Emphasis on Tropical Regions.

(b) Analyses of random interaction matrix models (RIMM) with group symmetries

(c) Relativistic coupled-cluster calculations

(d) SBDART (Santa Barbara DISORT Atmosphere Radiative Transfer)

In a nutshell, to cater the high end computational requirements and to adopt latest technologies, approximately every six-seven years, the Computer Centre has taken timely action to setup state of the art computing facility in PRL.

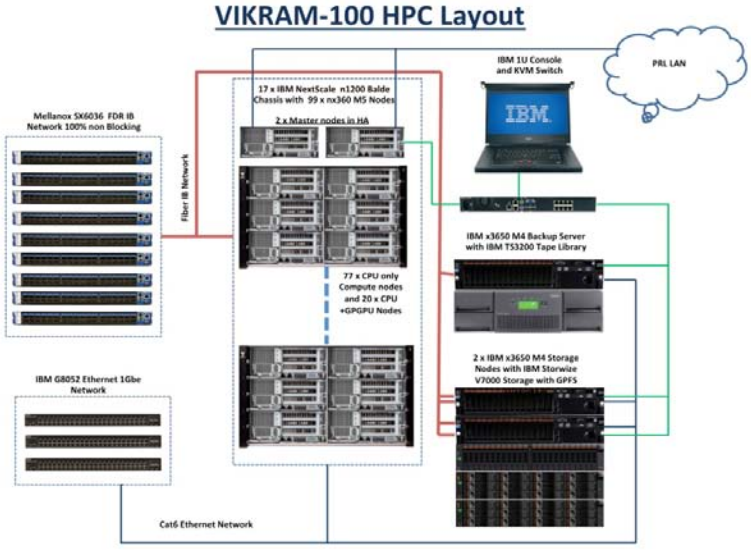


3. About 100TF High Performance Computing Cluster – Vikram-100

The VIKRAM-100 is a High Performance Computing (HPC) Cluster with 100 teraflops sustained performance. This is a centrally-run service to support scientists, researchers and research scholars at the Physical Research Laboratory (PRL) who require high performance computing. At installation, the Vikram-100 was the 13th fastest supercomputer in India *[Ref. http://topsc.cdacb.in/jsps/june2015/index.html]*. The facility was inaugurated by the Late Prof. U R Rao, Chairman, PRL Governing Council on Jun 26, 2015.

The Vikram-100 has 97 compute nodes, each with two Intel Xeon E5-2670v3 12-core Intel Haswell CPUs at 2.30 GHz, 256 GB RAM and 500 GB of local scratch storage. Twenty of these nodes also have two Nvidia Tesla K40 GPU cards and each card is capable of delivering 1.66 Tflops (double precision). The HPC has a global high performance parallel file system based 300 TB storage shared across all nodes. In brief, the 97 computing nodes of the Vikram-100 offers 2,328 CPU cores, 1,15,200 GPU Cores, 25 TB of RAM and 300 TB of high performance parallel file system.

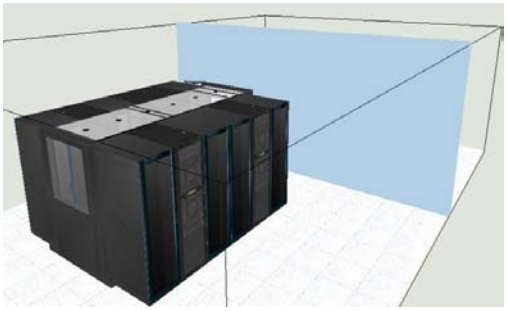
The Vikram-100 has an internal primary 100% non-blocking FAT Tree Topology FDR (56 Gbits/Sec) Infiniband Network for inter process communication between the compute nodes and for global shared storage. In addition, it has an internal secondary Gigabit Ethernet network for management and backup purposes. To provide un-interrupted power supply, UPS and Diesel Generator are also used. It has two High Availability (HA) master nodes where users login to compile, debug and submit jobs. Below figure shows an architectural overview of the Vikram-100 HPC facility.



100TF High Performance Computing Cluster – Vikram-100

Below figures show actual image of setup and figure-5 shows 3D view of HPC room.

Vikram-100 – HPC Live Setup



Vikram-100 3D View

The table below shows the software components available on the Vikram-100. All the software are installed as modules so that user can use suitable version as per their needs. More details are available on ***https://www.prl.res.in/prl-eng/hpc/vikram_hpc***

Sr. No.	Operating System/Software	Version
1.	Redhat Enterprise Linux	6.5
2.	Intel Parallel Studio XE 2015 – Cluster Edition	15.0.2 20150121
3.	Nvidia CUDA	6.5
4.	PGI Compilers	15.3
5.	Intel MPI	Version 5.0 Update 3
6.	IBM Job Scheduler and Management	4.2
7.	Open Sources Tools/Libraries like GCC, Gfortran, netcdf, nco, HDF, Lapack, BLAS, OpenMPI, glib	Based on users' need
8.	Scientific Software – Grid Mathematica, Comsol	-

4. Inauguration and Media Coverage

The Vikram-100 supercomputer facility was formally unveiled by Late Prof. U R Rao, chairman of PRL Council of Management on 26/June/2015. Few glimpses of the inauguration functions along with the media coverages are shown below.

Vikram-100 HPC Inauguration by Late Prof. U R Rao

Newspaper Coverage (27/June/2015):

(A) Indian Express


ENGLISH

Follow Us:

The Indian EXPRESS

Saturday, June 20, 2020

Home India Cities Opinion Sports Entertainment Lifestyle Tech Videos Explained Audio Real Estate Epaper Sign in

COVID19 India-China faceoff: Sonia asks questions, her Opp colleagues underline solidarity

Home / India / India Others / 13th fastest supercomputer in India inaugurated at PRL

13th fastest supercomputer in India inaugurated at PRL

Dilip Angom, who led the team in building this supercomputer at PRL said, "Christened as VIKRAM-100, this supercomputer is the 13th fastest supercomputer in India and is more powerful than 200 desktop computers."

(B) Gujarat Samachar


PRLમાં દેશનું સૌથી ઝડપી સુપર કમ્પ્યુટર 'વિક્રમ-૧૦૦' વિકસાવાયું

માત્ર દોઢ વર્ષમાં તૈયાર કરાયેલું 'વિક્રમ-૧૦૦' ૨૫૬ જીબી પ્રતિ નોડની મેમરી અને ૩૦૦ ટેરાબાઈટ્સની સ્ટોરેજ ક્ષમતા ધરાવે છે

કોરા કાગળો પર રૂપિયાની નોટો મૂકી લોકોને છેતરતા બે ગઠિયા ઝડપાયા

5. Scientific Applications

The Scientific and Technical fraternity of PRL have written their own codes/applications or collaborative code/application to run on Vikram-100. Few of them are

(a) A number of relativistic all-order atomic many-body methods in the Fock-space, equation-of-motion, normal and analytical response coupled-cluster theory frameworks are developed in-house at PRL. These methods are applied to study a number of fundamental physics including properties of atomic clocks, probing new physics beyond the standard model of particle physics, high-accuracy determination of atomic spectroscopy of plasma embedded atomic systems and investigating structures of atomic nuclei.

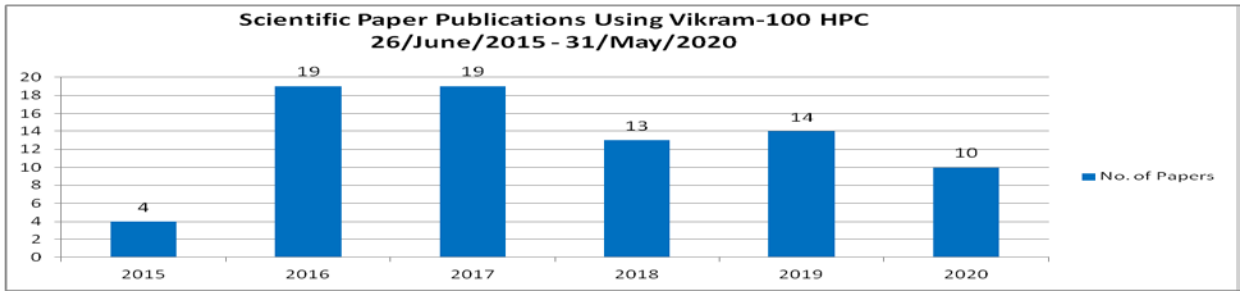
(b) Developed parallel codes to solve the single-site and cluster mean field theory models of strongly interacting ultracold bosons in optical lattices. Using these codes, it is possible to explore the quantum phase diagrams and quench dynamics. The results from these studies can shed light on the physics of the finite size quantum systems and their

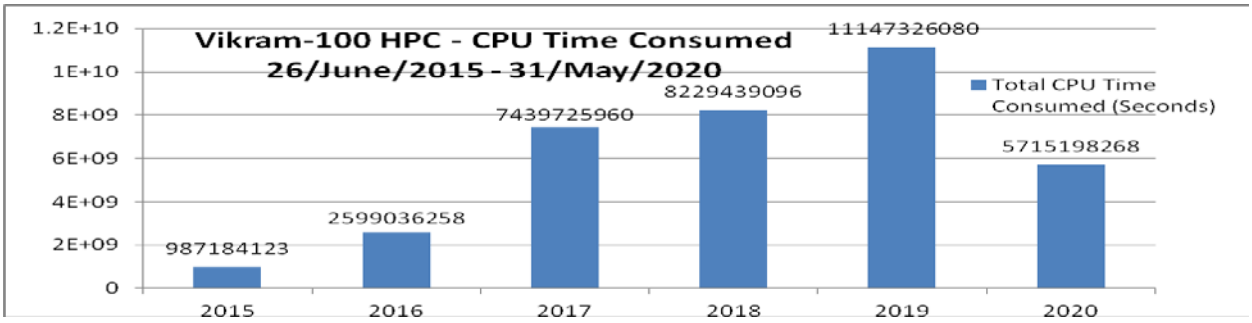
response to external perturbations. In addition, parallel codes for exact diagonalization method have also been developed.

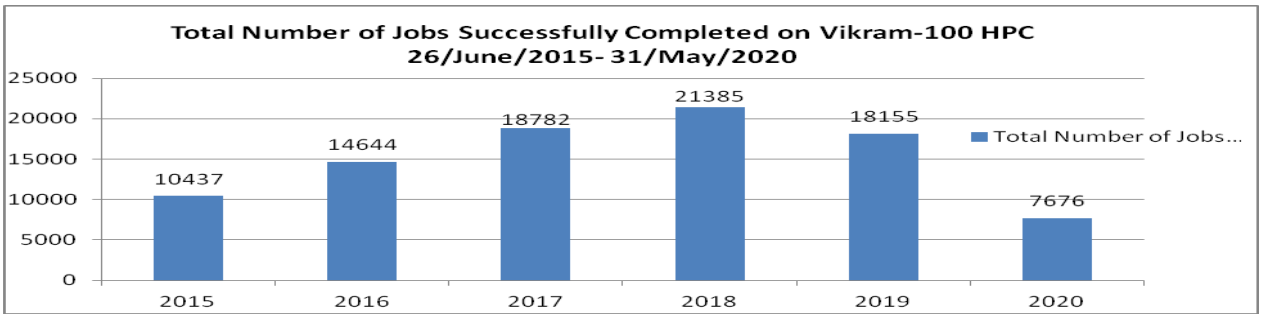
(c) To model the atmosphere of ultra-hot Jupiter. The computations perform on PRL Vikram-100 cluster is used to understand various physical and chemical process that occurs in the atmosphere of ultra-hot Jupiter.

6. Scientific Paper Publications and Usage Status

The high end computational facility is extensively used by PRL scientific and technical fraternity and as on May 31, 2020, a total of 77 scientific papers have been published in the national and international journals where Vikram-100 computational facility is acknowledged. In addition, there are several other scientific publications under review which are based on the results obtained from Vikram-100. The graphs below show (a) Year wise scientific paper publications (b) Yearly CPU usage and (c) Yearly total number of successful completion of jobs.







7. Testimonials

"The Vikram-100 HPC of PRL is providing excellent support for computationally extensive research program of PRL. This facility has been widely used by researcher from all domains of fundamental sciences being conducted by PRL, including, Astrophysics, Solar, Atmospheric, Space, Geo and Planetary Sciences, as well as Theoretical and Atomic and Molecular Physics. The scientists of PRL have also trained many research scholars using the Vikram-100 HPC, which has opened new vistas for them. Close to 80 scientific publications in reputed journals have been published using the HPC.

PRL look forward to continued excellence in science results based on computing power rendered by Vikram-100 HPC." **– Dr. Anil Bhardwaj, Director, PRL**

"My group have benefitted immensely from Vikram-100. We have used it to develop sophisticated parallel codes capable of solving complex quantum many-body systems. We have employed these to provide key insights on the strongly interacting ultracold bosons. Such studies are relevant to the emerging quantum technologies. All these are possible with the excellent tech support from Jigar and his team." **– Dr. Dilip Angom**

"In a competitive research environment nature and complexity of problems often depend on the available facility and Vikram-100 HPC gave us a remarkable opportunity to investigate the challenging ones. High energy physics group also working on some new directions using machine learning optimally using both CPU and GPU. Tech support is there always and awesome." **- Dr. Partha Konar**

"I use Vikram-100 HPC facility to run Lagrangian Particle Dispersion Model and Global Climate Model to understand the role of biomass burning in Earth's climate. These models are so complex and require such huge computational resources in terms of processing power and storage space, I can't even think of pursuing current research direction without Vikram-100 HPC." **– Dr. Harish Gadhavi**

"Vikram-100 HPC facility is my "lifeline", as I have used it extensively to run large GCMs (or Climate Models) to study the atmospheres of Earth and Mars. This has yielded results of high scientific value and I cannot imagine my work without the HPC cluster." **– Dr. Varun Sheel**

"I am using PRL Vikram-100 cluster to model the atmosphere of ultra-hot Jupiter. With its fast processing ability, allocations of operations and data across different units, I ould able to perform more computation efficiently. The computation perform on PRL Vikram-100 cluster is used to understand various physical and chemical process that occurs in the atmosphere of ultra-hot Jupiter." **- Dr. Arvind Singh Rajpurohit**

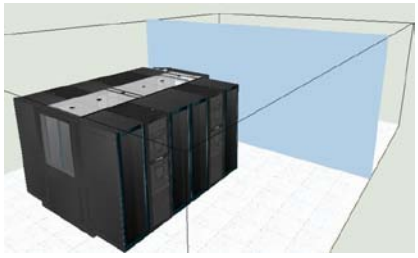
"We utilize Vikram HPC to perform modelling of atmospheric chemistry and dynamics with focus over South Asia. Our simulations provide valuable insights into the complex interplay of natural and man-made factors affecting the distribution of trace gases and aerosols. Our research, supported by the Vikram facility, also assists greatly in designing the new field experiments." ***- Dr. Narenda Ojha***

"During the era of High-Performance Computing (HPC), this teraflop machine is a boon to the researchers of PRL. Like other computational fields, Magneto hydrodynamic simulations also benefited from this machine. Vikram-100 has helped us develop, debug, and run state-of-the-art HPC codes in the field of Astrophysics and Solar Physics." ***– Dr. Aveek Sarkar***

"The Vikram-100 has been utilized for state-of-the-art numerical modeling and fundamental research related to various solar transients. Noteworthy are the high-resolution data-constrained modeling of solar flares which have recently been recognized by the international research community. Another important work is the simulation which showed that coronal heating can be due to dissipation of thin channels of current which are generated by chaotic magnetic fields. The work was showcased in the press release of the American Institute of Physics (AIP). Recently, an epidemiology model has also been established which utilizes the Vikram-100 cluster." ***- Dr. Ramit Bhattacharyya***

"A number of relativistic all-order atomic many-body methods in the Fock-space, equation-of-motion, normal and analytical response coupled-cluster theory frameworks are developed in-house at PRL. These methods are applied to study a number of fundamental physics including properties of atomic clocks, probing new physics beyond the standard model of particle physics, high-accuracy determination of atomic spectroscopy of plasma embedded atomic systems and investigating structures of atomic nuclei.." ***– Dr. Bijaya Kumar Sahoo***

8. Glimpses of Vikram-100 HPC Facility Preparation










9. Acknowledgement

We deeply thank Director, PRL for his continuous guidance for improving PRL Computational and Network facilities and encouragement for taking new initiatives. We thank Registrar, PRL for his kind support and guidance to improve IT facilities of PRL. We thank Prof. Angom Dilip Kumar Singh, Chairman, High Performance Computing Committee, Prof. Varun Sheel, Chairman, Computer Committee and Committee Members for their valuable guidance, feedback that always help us to setup a better Computational Facilities and Network Infrastructure. We also thank all our users for their valuable feedback, which always help us to improve our computational and networking facilities. We would like to thank all our Computer Centre colleagues. Without their continuous efforts, hard work with enthusiasm and teamwork helped Computer Centre to setup secure, reliable and efficient computational infrastructure. Last but not the least; we would like to thank all those who provided their help directly or indirectly in improving PRL Computational and Network facilities.

Appendix-I

Office Memorandum – 100TF HPC Committee

भौतिक अनुसंधान प्रयोगशाला
(अंतरिक्ष विभाग की यूनिट, भारत सरकार)
नवरंगपुरा, अहमदाबाद - 380 009, भारत
तार: रिसर्च फैक्स: 91-(0)79-26314900
दूरभाष: 26314000 ई-मेल: root@prl.res.in

Physical Research Laboratory
(A Unit of Dept. of Space, Govt. of India)
Navrangpura,Ahmedabad - 380 009, India
Cable: "RESEARCH" Fax : 91 - (0) 79 26314900
Phone: 26314000 E-mail : root@prl.res.in

Sr.AO/Committee-3/2013 December 16, 2013

OFFICE MEMORANDUM

Sub:- Formation of a committee to look into the technical aspects and acquisition of 100FLOP HPC Cluster.

The Director, PRL, constitutes the following Committee to examine the various aspects of the technical specifications related to the 100TELOP High Performance Computer to be acquired by PRL:

1.	Dr. Angom Dilip Kumar Singh	:	Chairman
2.	Dr. Varun Sheel	:	Member
3.	Dr. Bijaya Kumar Sahoo	:	Member
4.	Dr. Ramitendranath Bhattacharyya	:	Member
5	Mr. Samuel Johnson	:	Member
6.	Prof. R. Krishnan, IITM, Pune	:	External Expert
7.	Mr. Jigar A. Raval	:	Convener

The Committee after finalizing the technical specifications will submit the report to Director for approval.

Further, the committee, with or without the external expert as per norms, shall be associated with other official procedures related to the purchase of the cluster as and when required.

A.D. Mehta
16.12.2013
(Anand D. Mehta)
Senior Administrative Officer

To

All the Members of the Committee

Copy to: Director's Office/Registrar's Office/Head, Accounts/Senior Purchase & Stores Officer/Stores Officer.