HPC Resources of South Ural State University

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Abstract. Currently, South Ural State University (SUSU) has significant achievements in supercomputer modeling, artificial intelligence and Big Data. The high-performance resources of SUSU include an energy-efficient supercomputer "Tornado SUSU" and a specialized multiprocessor complex "Neurocomputer". The "Tornado SUSU" supercomputer and the "Neurocomputer" complex are at the center of the scientific life of the University and enable complex calculations for engineering, natural and human sciences, artificial intelligence. The high-performance resources of SUSU are used in education and for calculating the tasks of the University's partners. The paper describes the "Tornado SUSU" supercomputer and "Neurocomputer" complex technical features, system and application parallel software, scientific and engineering tasks solved with the help of the SUSU resources.

Keywords: Supercomputer · Neurocomputer · Parallel storage system · Supercomputer administration · Supercomputer modeling · Neural networks

1 Introduction

South Ural State University has achieved significant results in the field of digital industry creation. Research is actively developing with the use of supercomputer modeling, artificial intelligence and Big Data. Currently, SUSU has an energy-efficient supercomputer "Tornado SUSU", which ranks 15-th in the TOP50 list of the most powerful CIS supercomputers (September 2021). Tasks in the field of artificial intelligence require high parallelism on shared memory, however, a supercomputer with a cluster architecture does not provide it. To create artificial neural networks, SUSU acquired a specialized multiprocessor complex "Neurocomputer". The neurocomputer uses powerful advanced graphics accelerators to train neural networks. SUSU's high-performance computing resources are used by more than 500 people, these are not only employees and students of South Ural State University, but also employees of external educational, scientific and industrial organizations (industrial enterprises, universities, institutes of the Russian Academy of Sciences). SUSU established the Scientific and Educational Center "Artificial

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Intelligence and Quantum Technologies" (SEC AIQT) [32]. SEC AIQT employees are engaged in the administration of the high-performance resources of SUSU and scientific research in the field of supercomputer technologies, as well as provide user support.

The paper is structured as follows. Section 2 introduces the main high-performance SUSU resources installed in the SEC AIQT, such as the "SUSU Tornado supercomputer", the "Neurocomputer" complex, Panasas ActiveStor 11 data storage systems, OceanStor Dorado 3000 V6, Huawei OceanStor 5300 V5. Section 3 contains an overview of the system software used in the SEC AIQT. The application of equipment monitoring and control systems and software systems in the SEC AIQT is described. Section 4 presents the application software available to users of SUSU's high-performance resources and provides an overview of the scientific and engineering tasks being solved. Finally, Sect. 5 contains the final conclusions.

2 High Performance Resources

2.1 "Tornado SUSU" Supercomputer

The "Tornado SUSU" supercomputer is a fully liquid-cooled computing system with a performance of 473.6 Teraflops, ranked 19-th in the TOP50 list of the most powerful supercomputers in Russia (March 2022). Liquid cooling improves system energy efficiency (40–50% energy savings compared to air-cooled systems) and maximizes electronics packaging density. This makes it possible to get rid of moving parts in the computer, noise and vibration, thereby increasing the reliability and ergonomics of the system [1]. The technical features of the "Tornado SUSU" supercomputer are presented in Table 1.

The "Tornado SUSU" supercomputer is equipped with a high-performance parallel data storage system Panasas ActiveStor 11. It is designed to store initial data and user calculation results. Its peak performance is 30,886 IOPS, the write speed is 2402 MB/s, and the read speed is 3239 MB/s. Currently, more than 500 users of the supercomputer successfully use the storage; the system has been in continuous use since its installation in 2013 and has proven to be fault-tolerant and reliable.

The Panasas ActiveStor 11 storage system consists of five shelves. Four shelves contain 10 storage nodes (StorageBlade) with a capacity of 4 TB each and one control node (DirectorBlade), the fifth one consists of 11 storage nodes. The storage capacity is 204 TB, part of which is reserved for data replication. Control nodes perform the task of storing metadata and provide access to data using protocols such as NFS and CIFS. The system is configured with 7 virtual hot spare nodes, allowing to achieve operational stability in the case of a failure of up to seven disks inclusive.

The shelves in Panasas ActiveStor 11 only support the 10 Gigabit Ethernet interface. Three Panasas Ininiband routers are used to connect the system to the 40 Gb/s Infiniband QDR network, they route packets from the Infiniband QDR network to the storage network. Network load balancing is performed on compute nodes via routes to the storage system network with the same metric.

Table 1. Technical features of the "Tornado SUSU" Supercomputer

Technical features	Value
Quantity of compute nodes/ processors/coprocessors/cores	480/960/384/29184
Type of processor	Intel Xeon X5680 (Gulftown, 6 cores, 3.33 GHz)
Type of coprocessor	Intel Xeon Phi SE10X (61 cores, 1.1 GHz)
RAM	16.9 TB
Disk memory	204 TB, Panasas ActiveStor 11; 700 TB, Huawei OceanStor 5300 V5
System network	InfiniBand QDR (40 Gbit/s)
Control network	Gigabit Ethernet
Peak performance	473.6 TFlops
Operating system	Linux CentOS 6.2

2.2 "Neurocomputer" Complex

The architecture of the "Neurocomputer" complex is based on heterogeneous graphics accelerators. Thus, the "Neurocomputer" structure allows one to flexibly choose the appropriate equipment for the most efficient calculation of any task related to neural networks. The complex consists of six servers united by a common task queue, with the help of which the user gets access to the server with the architecture required for his task. The technical features of the "Neurocomputer" complex are presented in Table 2.

The architecture of the "Neurocomputer" complex is shown in Fig. 1 and consists of two Dell PowerEdge R750 GPU servers based on NVIDIA Ampere A100, three Dell PowerEdge R750 GPU servers based on NVIDIA Ampere A30, one HPE Apollo ProLiant XL270d Gen10 GPU server based on NVIDIA Tesla V100, and three Dell PowerEdge R640 management servers.

The Dell PowerEdge R750 GPU server features two NVIDIA Ampere A100 GPUs with 80 GB of VRAM, two Intel Xeon Silver 4314 processors, 192 GB of RAM and 1.9 TB of SSD storage. The Dell PowerEdge R750 GPU server based on NVIDIA Ampere A30 consists of two GPUs with 24 GB VRAM, two Intel Xeon Silver 4314 processors, 192 GB RAM and 1.9 TB SSDs. These servers are best suited for video-memory-demanding tasks and tasks that require exclusive access to the resources.

The HPE Apollo ProLiant XL270d Gen10 GPU Server is a server with eight NVIDIA Tesla V100 SXM2 GPUs (32 GB VRAM) connected by NVLink,

Table 2. Technical features of the "Neurocomputer" complex

Technical features	Value
Quantity of GPUs/ CUDA cores	18/91432
Types of GPUs	NVIDIA Ampere A100 80 GB PCI-E – 4 pcs. NVIDIA Ampere A30 24 GB PCI-E – 6 pcs. NVIDIA Tesla V100 SXM2 – 8 pcs.
Quantity of processors/cores	18/268
Types of processors	Intel Xeon Gold 6254 (Cascade Lake, 18 Cores, 4 GHz) – 2 pcs.; Intel Xeon Silver 4314 (Ice Lake, 16 Cores, 3.4 GHz) – 10 pcs.; Intel Xeon Silver 4214 (Cascade Lake, 12 Cores, 3.2 GHz) – 6 pcs.
RAM	1920 GB
Storage systems	700 TB, Huawei OceanStor 5300 V5; 46 TB, Huawei OceanStor Dorado 3000 V6 – Storage system based on Solid State Drives (SSD)
Communication network	Mellanox Infiniband QSFP28, Mellanox Infiniband SFP28, Gigabit Ethernet
Peak performance	276.4 TFlops
Operating system	Linux Centos 7.8

two Intel Xeon Gold 6254 processors, 192 GB of RAM, and 7.68 TB of SSDs in total. The server allows one to achieve maximum efficiency when parallelizing tasks on several graphics accelerators.

The complex also includes three Dell PowerEdge R640 control servers required to organize the operation of the complex. Each control server contains two Intel Xeon Silver 4214 processors and 256 GB of RAM.

Large data sets, which usually consist of many small files (images, audio and video files), are used to train neural networks. The Huawei OceanStor Dorado 3000 V6 data storage system based on solid state drives is connected to the "Neurocomputer" complex. The storage system provides maximum performance when working with files for training neural networks. This storage system performs reads, writes two orders of magnitude faster than hard drives and does not lose performance when working with a many small files.

Huawei OceanStor Dorado 3000 V6 contains two controllers that can replace each other in the event of a failure of one of them, thus ensuring uninterrupted storage operation. Each controller has one Kungpeng 920 processor and an Ascend 310 coprocessor. The processor is developed by Huawei on top of the ARM architecture, with 96 GB of cache memory. The coprocessor is designed to support service neural networks built into the storage.

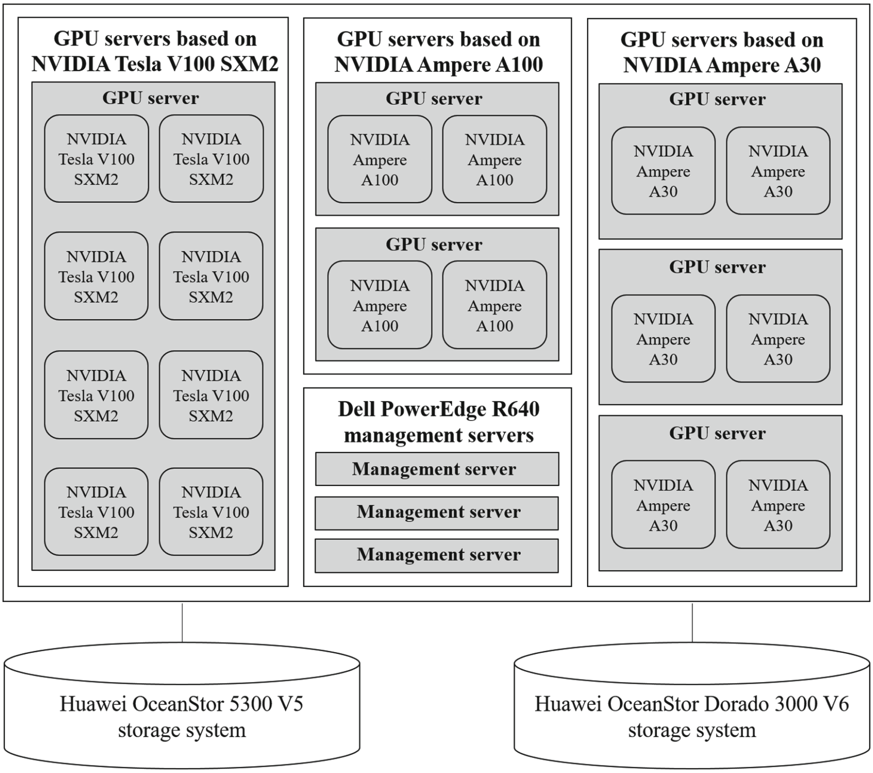

Fig. 1. Architecture of the "Neurocomputer" complex

The storage includes 12 Enterprise SSDs of 3.84 TB each. All storage components are Huawei's own design. The storage capacity is 46.08 TB with 192 GB cache memory. The effective amount of storage that users can use for their data is at least 35 TB, the rest of the space is used for storage fault tolerance.

The "Neurocomputer" complex uses the Huawei OceanStor 5300 V5 data storage system with 700 TB for long-term storage of user data and calculation results. The Huawei OceanStor storage architecture contains two controllers, each controller has one Kungpeng 920 processor with 64 GB of cache memory, data mirroring between the controllers is carried out via a 100 Gb/s network. The storage system includes 50 NL-SAS hard drives, 14 TB each. Support for the most popular protocols, such as NFS, CIFS, iSCSI, etc., makes it possible to use this storage for both the "Neurocomputer" complex and the "Tornado SUSU" supercomputer.

3 System Software

The CentOS 6.2 operating system is installed on each compute node of the "Tornado SUSU" supercomputer. Compilers such as Intel Compiler (C/C++, Fortran 77, Fortran 90), GCC, the MPI2 parallel programming library (Intel MPI, OpenMPI, MVAPICH) are used. They allow users to implement their own applications to solve their tasks.

The "Neurocomputer" complex has the CentOS 7.8 operating system installed. Users use several versions of the GCC compiler, the CUDA, NCCL and CUDNN libraries for working with graphics accelerators, the OpenMPI parallel programming library. The Anaconda system is installed on the "Neurocomputer" complex. It is used for configuring the user environment of the Python program (installing the required version of Python, installing related libraries that provide interaction with artificial neural networks, Keras [13], Tensorflow [34], etc.). A fault-tolerant and scalable cluster management and job scheduling system SLURM [27] is installed on each computer complex for the efficient sharing of resources by a many users. SLURM version 2.5.3 is installed on the "Tornado SUSU" supercomputer, SLURM version 20.02.4 is used in the "Neurocomputer" complex.

3.1 Monitoring Systems

One of the main tasks of a system administrator is to ensure the correct and uninterrupted operation of the equipment, for example, the Infiniband and Ethernet networks, data storage systems, etc. The Nagios and Zabbix systems are used for system monitoring at the Scientific and Educational Center "Artificial Intelligence and Quantum Technologies" (SEC AIQT). We also developed our own supercomputer load monitoring system. It is designed to generate reports on the load and activities of users from the structural divisions of the university [15].

The *Nagios* system provides information about the health of hardware and software services and generates a status change message sent by e-mail to the administrator [5]. The main approach to writing checks in Nagios is the description of checks in the form of scripts using a self-written code, as well as using a standard set of basic checks that are not suitable for organizing monitoring of all resources. Nagios gives the flexibility to perform checks on various services by allowing one to write simple checks yourself; however, this is also a serious drawback. You must independently describe all non-standard checks that require you to analyze the SNMP commands of the equipment. Notification via e-mail is also an inconvenient mechanism since letters often get into the spam folder or arrive later than necessary to respond quickly to problems. We use Nagios to check the status of services such as mail, task queues, networking, communications, and other types of the equipment (Fig. 2).

The Zabbix [6] monitoring system started to be used later than Nagios, but we use it more widely, since Zabbix has the ability to monitor systems actively and passively. In addition, it can be installed on Windows and Linux. Zabbix

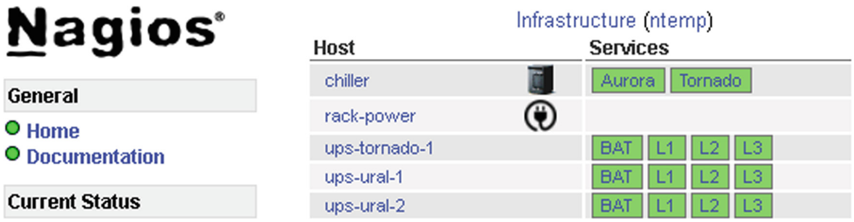

Fig. 2. Monitoring the equipment status using the web interface of the Nagios system

allows creating graphs for individual groups of the equipment (Fig. 3). It has a large and growing base of standard equipment checks (for example, for the Dorado storage system, etc.). This feature of Zabbix enables the setup of new equipment monitoring in the short term.

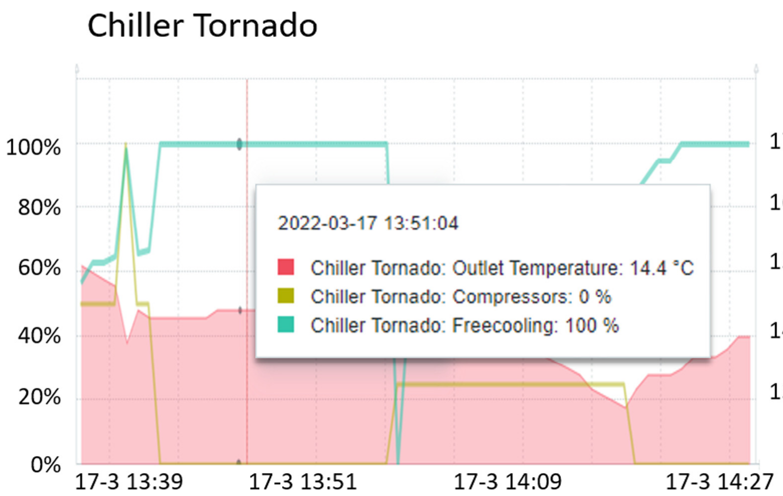

Fig. 3. Monitoring the state of the chiller of the "Tornado SUSU" supercomputer using the web interface of the Zabbix system

Graphs are also a useful Zabbix tool, they allow comparing parameters that have been monitored at different time intervals, identifying dependencies and problems. In addition to the above, a significant advantage of the Zabbix system is the ability to integrate with popular instant messengers and corporate systems, which enables to achieve almost instant response to a change in the state of the equipment or software service. Currently, Zabbix is being actively implemented. It replaces most of the functionality of Nagios, however, the Zabbix system cannot fully cover the functionality of Nagios yet. The SEC AIQT infrastructure diagram in the Zabbix monitoring system is shown in Fig. 4.

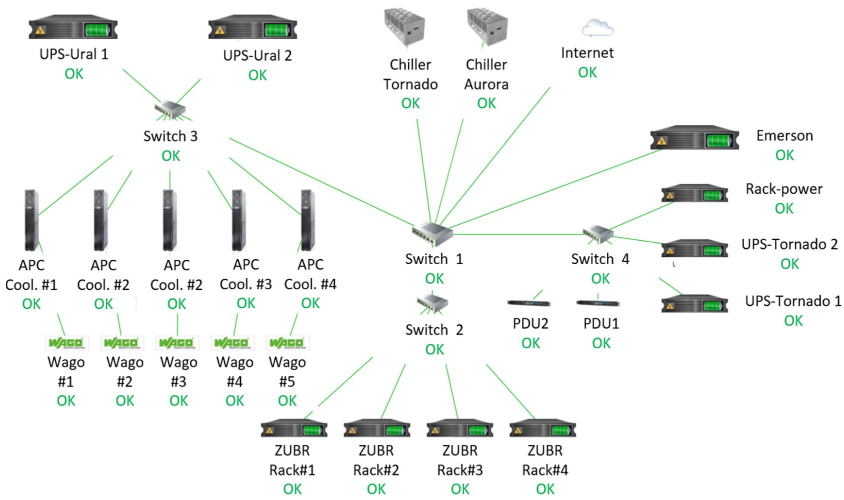

Fig. 4. SEC AIQT infrastructure diagram in the Zabbix monitoring system

3.2 Control Systems

We use specialized software control systems, xCAT and Puppet, to install and configure software on a many compute nodes of the "Tornado SUSU" supercomputer.

xCAT (Extreme Cluster Administration Tool) is a scalable toolkit for deploying and maintaining large clusters [18]. xCAT provides a unified interface for hardware management, the discovery and deployment of diskful/diskless operating systems. All commands are client-server, logged and controlled by policies. They also support authentication. xCAT supports the differentiation of rights based on access policies. The entire flow between the client and the server in the xCAT client/server application is controlled by the xcatd service (xCAT daemon) on the Management Node. When the xcatd service receives an XML-packaged command, it checks the sender's credentials against the ACLs in the policy table.

The service also receives information about the state and status of the nodes from the moment they start working. xCAT is designed to scale very large clusters. Hierarchy support allows one control node to have any number of stateless or stateful service nodes, which improves performance and enables the management of very large clusters. xCAT is used for installing a clustered operating system on compute nodes, by PXE booting over DHCP, with the initial installation and configuration of the operating system, and running the Puppet system background process for further configuration.

Puppet is a configuration management system and a language for describing configuration tasks. System administrators use Puppet to effectively manage a many systems and ensure a single configuration. We set up all compute node configurations with Puppet after its basic installation with xCAT. Namely, we install SLURM task queues, packages for working with the high-speed

Infiniband network, storage and system packages. This organization of the system installation enables to make changes to the system configuration if necessary.

4 Application Software

The high-performance computing resources of SUSU have both proprietary and free application software installed [33], including:

- ANSYS, CAE/multiphysics engineering simulation software for product design, testing and operation [3];
- LS-DYNA, a general-purpose multiphysics simulation software package [19];
- FlowVision, complete, integrated CFD software [9];
- SFTC DEFORM, engineering software that enables designers to analyze metal forming, heat treatment, machining and mechanical joining processes on the computer [25];
- MATLAB, a programming and numeric computing platform used by millions of engineers and scientists to analyze data, develop algorithms, and create models [20];
- OpenFOAM, free, open source CFD software. It has a large user base across most areas of engineering and science, from both commercial and academic organizations [24].

More than 250 scientific tasks are annually performed on the computing resources of SUSU. These are tasks from the fields of artificial intelligence, mechanical engineering, metallurgy and metalworking, the fuel and energy complex, light industry, the production of supercomputers and software, including:

- forecast of the passage time of the queue of highly automated vehicles based on neural networks in the services of cooperative intelligent transport systems [26]
- tigris basin landscapes: sensitivity of the ndvi vegetation index to climate variability derived from observation and reanalysis data [2]
- simulation of the compressibility of isostructural halogen containing crystals on macro- and microlevels [4],
- quantum electronic pressure and crystal compressibility for magnesium diboride under simulated compression [21],
- reaction mechanism and energetics of the decomposition of tetrakis-(1,3-dimethyltetrazol-5-imidoperchloratomanganese(II)) from quantum-mechanics-based reactive dynamics [36],
- ab initio calculation of the total energy of a bcc iron cell containing three dissolved carbon atoms, and internal friction in Fe–C solid solutions [23],
- duplexer based on volumetric modular technology [10],
- VaLiPro: linear programming validator for cluster computing systems [29],
- A parallel computation model for scalability estimation of iterative numerical algorithms on cluster computing systems [28],
- in-RDBMS industrial sensor data analysis [39],

- parallel similarity search [16] and discovery of time series motifs [40], anomalies [38,41], and snippets [37],
- aramid fabric surface treatment and its impact on the mechanics of the frictional interaction of yarns [11],
- development of a supercomputer model of needle-punched felt [7],
- plastic deformation at the dynamic compaction of aluminum nanopowder: molecular dynamics simulations and mechanical model [22],
- micromechanical model of representative volume of powder material [12],
- towards the fog computing PaaS solution [35],
- fog computing state of the art: concept and classification of platforms to support distributed computing systems [14],
- transfer learning for Russian speech synthesis [17],
- model of compound eye vision for machine learning [30],
- student attendance control system with face recognition based on a neural network [31],
- traffic flow estimation with data from a video surveillance camera [8].

5 Conclusions

In this article, we reviewed the high-performance resources of South Ural State University, i.e., the "Tornado SUSU" supercomputer, the "Neurocomputer" complex, the Panasas ActiveStor 11 data storage systems, OceanStor Dorado 3000 V6, Huawei OceanStor 5300 V5. Access to the resources is provided by the Scientific and Educational Center "Artificial Intelligence and Quantum Technologies" established at SUSU. Currently, the HPC resources are used by more than 500 people. These are students and employees of SUSU and external educational, scientific and industrial organizations. Employees of the SEC AIQT maintain the operability of the SLURM task queue, ensure the correct and uninterrupted operation of the Infiniband and Ethernet networks, storage and other equipment using specialized monitoring and management systems. Modern parallel software is installed on the high-performance resources of SUSU, which allows performing research and development work from different fields of knowledge.

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