SUSU Supercomputer Resources for Industry and Fundamental Science

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***Abstract*—The supercomputers of South Ural State University are at the core of the University's research performance. These facilities enable researchers to perform a broad range of computationally demanding tasks in the fields of engineering, natural and human sciences, and IT. The powerful capabilities of SUSU supercomputers are currently used for more than 250 research projects, including commercial projects as part of the Industry 4.0. The first-class facilities are ranked among the world's most powerful supercomputers by various ranking agencies.**

***Keywords*—supercomputer center, computing cluster, supercomputer simulation, parallel data-storage system, monitoring**

I. Introduction

The direction of supercomputing is actively developed in the South Ural State National Research University. The Supercomputer Simulation Laboratory (SSL) of SUSU has modern Russian supercomputers. There are more than 400 registered users on supercomputers of SUSU. The supercomputer capacities of the South Ural State University are fully loaded due to the large number of users. Supercomputers use modern imported and Russian parallel software: ANSYS CFX, Fluent, ANSYS Multiphysics, Maxwell, FlowVision, OpenFOAM, LS-DYNA, SFTC DEFORM, MathWorks MATLAB, etc. to provide access to the supercomputers of SUSU for the widest range of users and conduct their research. Currently, more than 250 scientific studies are performed on supercomputers of SUSU.

II. Supercomputers

SUSU regularly upgrades and extends its supercomputers to solve an ever-expanding range of industrial and scientific tasks. Now, the Supercomputer Simulation Laboratory of the South Ural State National Research University performs calculations using 3 supercomputers: Tornado SUSU, SKIF-Aurora SUSU, SKIF Ural. The dynamics of productivity growth of supercomputers of SUSU is shown in fig. 1. Computing cluster "SKIF Ural" with a peak performance of 16 Teraflops was developed by the Russian company T-Platforms in 2008. The next supercomputer "SKIF-Aurora" was developed in 2011 by the Russian company RSC SKIF together with the Program Systems Institute of RAS and has a performance of 117 Teraflops. The company RSC-Technologies developed the most powerful supercomputer "Tornado SUSU" with a performance of 473 Teraflops in 2013.

The "SKIF Ural" compute cluster based on an air cooling system, while the supercomputers SKIF-Aurora and Tornado SUSU based on full direct liquid cooling system. It allowed to reduce the area of premises required for placing computer complexes and in addition to achieve high energy efficiency of supercomputers.

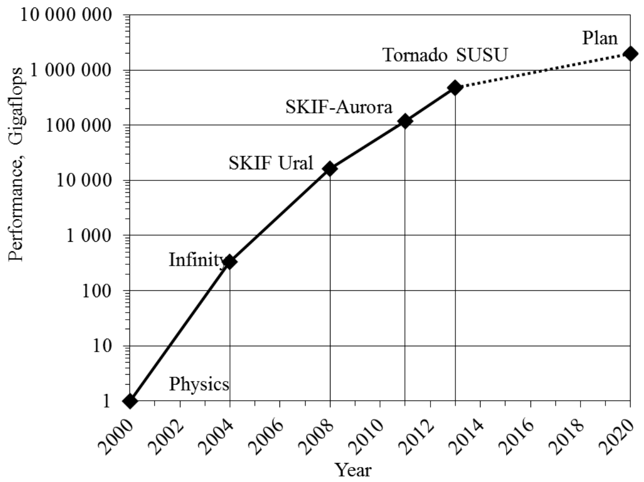

Fig. 1. The supercomputer center's dynamics of development of computing resources

A. Supercomputer "Tornado SUSU"

Supercomputer Tornado SUSU with a performance of 473 Teraflops takes the 8th place in the CIS ranking TOP50 (April 2018). Supercomputer has full direct liquid cooling, the highest density of packaging of electronic components and energy efficiency. The supercomputer consists of 480 two-processor computing nodes based on Intel Xeon processors and manycore accelerators (see Table 1). In 2013, Tornado SUSU was the first non-US computing installation to use multi-core Intel Xeon Phi accelerators.

TABLE I. CHARACTERISTICS OF THE SUPERCOMPUTER TORNADO SUSU

Number of computational nodes/ processors / coprocessors / cores	480/960/384/29184
Processor	Intel Xeon X5680 (6x3.33 GHz) – 960 pcs.
Type of coprocessor	Intel Xeon Phi SE10X (61x1.1 GHz) – 384 pcs.
Memory	16.9 TB
Disk storage	300 TB on a parallel storage system Panasas ActiveStor 11 and on SSD drives
Type of system network	InfiniBand QDR (40 Gbps)
Type of control network	Gigabit Ethernet
Peak performance of the complex	473.6 Teraflops
Performance of the complex on the LINPACK	288.2 Teraflops
Operating system	Linux CentOS

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B. *Supercomputer "SKIF-Aurora SUSU"*

The supercomputer "SKIF-Aurora SUSU" is a complex solution that was developed by the company RSC SKIF with the participation of the Program Systems Institute of RAS in 2010. The supercomputer SKIF-Aurora SUSU consists of 736 compact and powerful computing blades with liquid cooling (see Table 2). Now the system occupies the 20th place in the rating of the most powerful supercomputers of the CIS TOP50.

TABLE II. CHARACTERISTICS OF THE SUPERCOMPUTER "SKIF-AURORA SUSU"

Number of computational nodes / processors / coprocessors / cores	736/1472/8832
Processor	Intel Xeon X5680 (6x3.33 GHz)
Memory	3 TB
Disk storage	64 TB SSD
Type of system network	3D Torus (60 Gbps, 1 µs latency)
Type of control network	InfiniBand QDR (40 Gbps, 2 µs latency)
Service Networks	Service Network SKIF ServNet v.4 Global Synchronization Network
Accelerators	Programmable FPGA Accelerators
Peak performance of the complex	117 Teraflops
Operating system	Linux CentOS

C. *Computing cluster "SKIF Ural"*

The high-performance computing cluster "SKIF Ural" was developed by T-Platforms for SUSU within the framework of the Priority national project "Education" in 2008. The cluster consists of 168 computational nodes (see Table 3). The cluster is no longer a top class system currently, and it is used for students' education in the framework of the Personal Virtual Computer (PVC platform) VDI-system. Within the framework of the PVC platform, a PVC based on Windows with personal profile is created for each user. PVC is a universal means of access for a student to the cloud of educational services of the university, based on the infrastructure of virtual desktops and applications. Students use personal laptops, netbooks, tablets or other devices to run PVC. As a result, any classroom of university with workstations equipped with electrical outlets can be used as a computer class.

TABLE III. CHARACTERISTICS OF THE SKIF URAL COMUTE CLUSTER

Number of computational nodes / processors / coprocessors / cores	166/332/1328
Processor	Intel Xeon E5472 (4 cores at 3.0 GHz)
Memory	1.33 TB
Disk storage	49.29 TB
Storage System	Panasas ActiveStor 5100 (20 TB)
Type of system network	InfiniBand DDR (20Gbit/s)
Type of control network	Gigabit Ethernet
Service network	SKIF ServNet
Peak performance of the complex	16 Teraflops
Performance of the complex on the LINPACK	12.2 Teraflops
Operating system	Windows HPC Server

III. PARALLEL STORAGE SYSTEMS

The supercomputers of SUSU use various storage systems (data storage systems), which were produced by companies Panasas, HP and AXUS.

A. *Panasas ActiveStor 11 Parallel Storage System*

The supercomputer "Tornado SUSU" was initially equipped with the AXUS YB storage system, on the basis of which the Lustre file system was configured. With a small number of nodes and users working on a supercomputer, Lustre coped with the load, and the work was fairly stable. With the growing number of supercomputer users, storage performance has become scarce. The high-performance parallel storage system Panasas (2 shelves, 22 blades) was installed in the supercomputer Tornado SUSU in 2013, and the AXUS YB storage system was used to store service data, such as distributions, package repositories, etc. Later, AXUS storage was reconfigured to work with CIFS. At present, Panasas storage system on the Tornado SUSU supercomputer consists of 5 shelves, united in a single system. Four shelves each contain 10 storage servers (StorageBlade), each has a capacity of 4 TB and one management server (DirectorBlade), the fifth shelf contains 11 storage servers. The total storage capacity is 204 TB, but in fact it is smaller, because part of the storage servers is used for data replication. The system is configured to 7 hot spare virtual nodes, allowing to keep the system in working order upon failure of up to 7 data storage blades. The DirectorBlade nodes serve to store metadata and run services on them to provide access to data, such as PanFS, NFS and CIFS. Storage in the current configuration provides up to 30,000 IOPS in peak (see Table 4).

TABLE IV. CHARACTERISTICS OF ACTIVESTOR 11 STORAGE SYSTEM

Characteristic	Average	Maximum
I / O Operations Per Second (IOPS)	6 115	30 886
Recording speed (MB/s)	245	2 402
Reading speed (MB/s)	213	3 239

The Panasas storage shelves support only 10 Gigabit Ethernet. To connect the storage system to the InfiniBand QDR cluster network, there are three InfiniBand routers Panasas, which routes packets from the network InfiniBand to the storage system. The scheme of connecting the storage system to the supercomputer "Tornado SUSU" is shown in fig. 2. Each of the five storage shelves is connected by 10-gigabit cables to the switch. The switch is connected by three pairs of the 10 GE cables with three InfiniBand-Panasas routers. InfiniBand routers are connected via 40-gigabit cables to the InfiniBand network of the supercomputer Tornado SUSU.

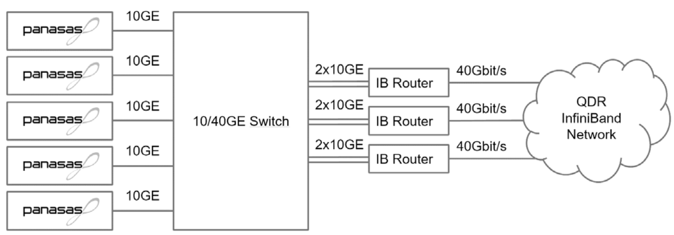


Fig. 2. Scheme of connecting Panasas ActiveStor 11 to the "Tornado SUSU" supercomputer network

Panasas ActiveStor is used to store the data and results of calculations of users of the supercomputer "Tornado SUSU". More than 400 users successfully use the storage system now.

B. Data Storage System AXUS YB-III Based On Lustre

Now there are two AXUS YB-III parallel storages. One storage is connected to the supercomputer "SKIF-Aurora", and the other to the Tornado SUSU. Each storage consists of 4 shelves, each shelf is integrated into an array RAID 10. The total capacity of each storage is 64 terabytes. The advantages of these storage facilities include high reliability of the hardware (for 7 years of intensive use, 1 of 16 power supplies and 4 of 128 Enterprise SATA hard disks are out of order.). The storage bottleneck is the parallel file system Lustre, which has lower reliability and performance than the commercial analogs. The performance of parallel storage, which is based on AXUS storage and file system Lustre, was 5000 IOPS in peak. This had limited the performance of the supercomputer severely. In addition, when file system errors occurred, they required a complete stop of all calculations until the process of fixing these errors was complete. Currently, the storage based on AXUS YB reconfigured and used to working with CIFS.

The logical scheme of connecting the AXUS storage system to the supercomputer Tornado SUSU is shown in fig. 3. Each storage shelf (Shelf-1 - Shelf-4) is divided into two parts. One part is formatted as the Ext4 file system. The parallel Lustre file system operates on the basis of this file system. The other part is used by the LVM (Logical Volume Manager) system, which treats these parts as physical volumes. Physical volumes are combined in Virtual Group Storage, which allows you to work with the storage as a single disk space. This virtual group is divided into two logical volumes, one of which is used to work with CIFS, and the other is configured as iSCSI.

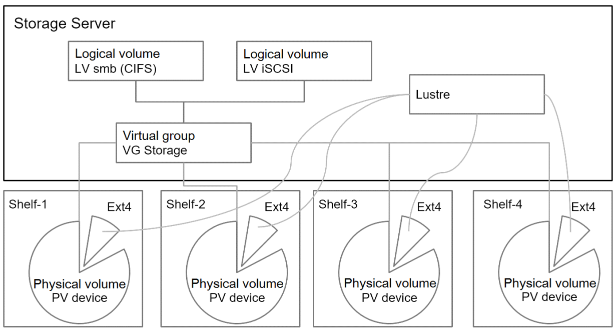


Fig. 3. Logical scheme of connecting AXUS storage system to supercomputer Tornado SUSU

C. Panasas ActiveStor 8 Parallel Storage System

Parallel storage system Panasas ActiveStor 8 proved to be a system with the highest reliability for eight years of use in the supercomputer "SKIF Ural". The reliability of the old Panasas ActiveStor 8 system was significantly higher than Panasas ActiveStor 11, acquired in 2013. The connection scheme of Panasas ActiveStor 8 to the supercomputer "SKIF Ural" is shown in fig. 4. Each of the two storage shelves is connected by four gigabit cables to a gigabit Ethernet switch, which is also connected to each of the 168 nodes of the "SKIF Ural" supercomputer.

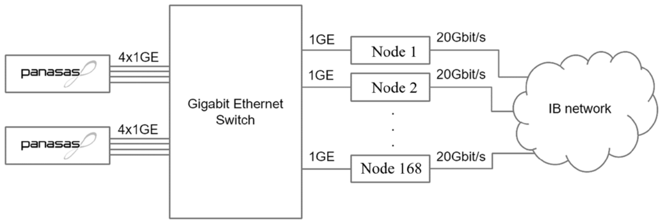


Fig. 4. Scheme of connecting Panasas ActiveStor 8 to the supercomputer SKIF Ural

IV. MONITORING SYSTEMS

Monitoring systems occupy an important place in modern computing centers [1], [2]. Supercomputer Simulation Laboratory of SUSU used a lot of monitoring systems, complementing each other. Both widely used open source and self-developed systems are used [3].

A. Open source Monitoring Systems

Nagios. Information about the most important services is displayed on the monitor, which is located on the wall in the hall of system administrators of the supercomputer center. The system allows staff to respond quickly to emerging technical problems. Administrators receive email notifications about service failures in their area of responsibility. Nagios allows you to get only general information about the operation of services by the type "works / does not work". Administrators use additional monitoring systems [4] to diagnose a specific problem.

Ganglia. Monitoring load computing cluster nodes is performed using the system. You can view the history, compare load compute nodes and look for reasons for the decline of computing performance [4].

Built-in monitoring systems are used in many ways by modern server equipment, for example, Panasas parallel storage system (see Figure 5), HP storage, APC infrastructure manager, monitoring system for chillers and air conditioners, etc. These built-in monitoring systems transmit information about their condition as a special SNMP (Simple Network Management Protocol) packets on the Nagios server, which is already involved in its further processing and shipment.

B. The Monitoring System of Supercomputer Center

Our own system of load monitoring SUSU supercomputers was developed in the Supercomputer Simulation Laboratory. The development of the system was caused by the necessity for regular creation of a set of specific reports about supercomputers' loading and activities of the structural unit of the university. When there are new requirements for reports, the procedure for generating additional statistical samples and graphs is added into the system's functionality. In the future, re-create the same report is faster and easier. Using this system, system administrators generate reports on the loading of supercomputers. They can view information about users and their calculations on a supercomputer, about the current load of clusters, the number of tasks in the queue, information about working and non-working nodes. It is also possible to generate reports on the loading of supercomputers automatically for a certain period. The ordinary users of the supercomputer can find information about free nodes in the queue, about the tasks of the user, both completed and running [3].

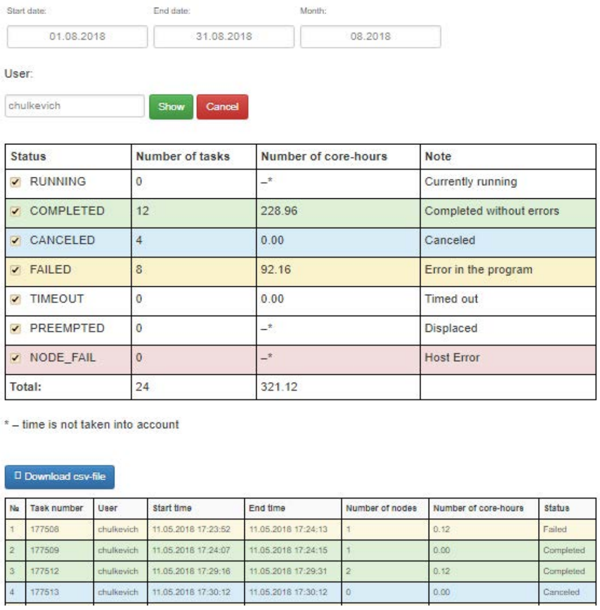
Fig. 5. Load monitoring system

The task queue SLURM, installed on the cluster, uses the MySQL database to store information about tasks that are already calculated or just added to the queue. The database contains information about the task number, the user who put the task on the calculation, the time of the task was queued, the number of the requested nodes, the start time and the end time of the task execution, and the status with which the task was completed. The module, written using the Django framework, is responsible for displaying information and visualizing data on loading supercomputers to the end user. Because Django is based on MVT (Model-View-Template) technology, it allows to quickly develop flexible Web applications, focusing directly on implementing the internal logic of the application.

The main page of the system (see Figure 5) contains the most important information which interests the director and administrators of the SSL SUSU, for example:

- statistics on the nodes as a percentage (working, off, reserved, free);
- statistics of the requested nodes in the queue (the number of nodes on which the work is already started, the nodes requested at the current time, blocked nodes and nodes that are released and will soon return to the queue);
- users who are "online" at the moment. That is, users who have already started the remote access terminal and are working in it now;
- load dynamics of supercomputer for a certain period;
- output the console command "sudo squeue", showing detailed information about all tasks currently running with the task queue (executed, pending, completed).

When there are new requirements for reports, the procedure for generating additional statistical samples and graphs is considerably simplified. For example, in fig. 6 shows an example of output information about the current and completed calculations of the selected user of the supercomputer for the specified period.


Start date: 01.08.2018 End date: 31.08.2018 Month: 08.2018

User: chulkevich Show Cancel

Status	Number of tasks	Number of core-hours	Note
RUNNING	0	–*	Currently running
COMPLETED	12	228.96	Completed without errors
CANCELED	4	0.00	Canceled
FAILED	8	92.16	Error in the program
TIMEOUT	0	0.00	Timed out
PREEMPTED	0	–*	Displaced
NODE_FAIL	0	–*	Host Error
Total:	24	321.12	

* – time is not taken into account

Download csv-file

№	Task number	User	Start time	End time	Number of nodes	Number of core-hours	Status
1	177508	chulkevich	11.05.2018 17:23:52	11.05.2018 17:24:13	1	0.12	Failed
2	177509	chulkevich	11.05.2018 17:24:07	11.05.2018 17:24:15	1	0.00	Completed
3	177512	chulkevich	11.05.2018 17:29:16	11.05.2018 17:29:31	2	0.12	Completed
4	177513	chulkevich	11.05.2018 17:30:12	11.05.2018 17:30:12	0	0.00	Canceled

Fig. 6. Information about the current and completed calculations of the selected user

- multiprocessor database machines with hierarchical architecture[9]-[13]
- simulation and analysis of hierarchical multiprocessor database systems [14]-[17];
- increasing efficiency of data transfer between main memory and various coprocessors [18], [19];
- properties of new boron phases [20];
- chemical processes in fuel cells [21], [22];
- chemical reactions at the Li solid state electrolyte [23];
- mechanical properties of thermoelectric materials [24]-[29];
- properties of amorphous Ni-Nb-Zr membranes [30];
- assessment of the conformity of protective devices roll-over protective structure (ROPS) to the requirements of passive safety [31];
- integration of DBMS and parallel data mining algorithms for Intel MIC processors [32], [33];
- encapsulation of parallelism into open-source DBMS [34], [35];
- very large graph partitioning on computer cluster [36], [37];
- parallel frequent pattern mining on Intel MIC processors [38];
- parallel clustering on Intel MIC processors [39], [40];
- parallel subsequence similarity search [41]-[43];
- sticker detection during continuous steel casting based on the use of Deep Neural Networks [44];
- the crystal structure modeling, the quantum chemical calculations and the stiffness tensor analysis were performed to explain and predict the mechanical

properties of promising crystalline materials including amino acid compounds [45];

- the feasible quantitative tools that based on calculated electronic properties of molecules and organic crystals were suggested for the chalcogen and halogen bonds categorizing [46]-[48];
- the calculations of theoretic Raman spectra and prediction of nonlinear optical properties of organic iodine-derived crystalline compounds were carried out [49]-[52];
- finite element modeling of uniformly compressed plates perforated in triangular patterns [53];
- finite element modeling of cold-formed steel channels with solid and slotted webs in shear [54]-[57];
- studying the non-Newtonian properties and rheology of lubricant in hydrodynamic journal bearings [58]-[60];
- solving a thermohydrodynamic lubrication problem for complex-loaded bearings [61];
- modeling in optical properties of carbon nanotubes[62], [63];
- modeling in alkali metals adsorption on carbon nanotubes [64], [65];
- modeling in atomic structure and mechanical properties carbon nanotubes [66];
- modeling in mechanics of composite materials [67], [68];
- assessment of the conformity of protective devices Roll-over protective structure (ROPS) to the requirements of passive safety [69];
- modeling of the working process in rocket engines [70]-[73];
- investigation of physical mechanisms and modeling of the effect of controlled vibration on the stabilization of the required geometry of dispersed particles in the dimensional dispersion of condensed media [74], [75];
- optimization of the design of electric vibration drives based on the switched-inductor motor and modeling of their work [75]-[77];
- fundamental research on distributed and grid-systems [78], [79].

V. Acknowledgment

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VI. Conclusion

Supercomputer technologies occupy a central place in the development programs of the South Ural State University. Supercomputers are equipped with modern domestic and imported parallel software with which the university research groups perform advanced research. To ensure the continuous operation of three supercomputers, four parallel data storage systems and numerous auxiliary services, the staff of the Supercomputer Simulation Laboratory use automatic monitoring systems that are able to automatically generate reports on the state of equipment and send them to the administrators and the director's mail.

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