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Research on the Construction and Management of High Performance Computing in Universities

Yizhi Zhang[1,a], Jinming Chang[1,b,*], Zhongling Ma[2,c]

[1]Shaanxi Normal University, Xi'an, China
[2]Northwest University, Xi'an, China
[a]yzzhang@snnu.edu.cn, [b]dyjdcs@126.com, [c]xdmzl@nwu.edu.cn
**Corresponding author*

Abstract: *With the widespread use of high performance computing in scientific research and the addition of artificial intelligence and big data related majors in colleges and universities in recent years, the demand for computing power of high performance computing in colleges and universities is getting higher and higher. As a result, many universities have problems such as scattered computing resources, repeated construction, inadequate computing power, complicated operation and maintenance, and many security risks. How to give full play to the core potential of high performance computing resources is an urgent task. The article discusses how to improve the efficiency of using high performance computing resources in universities to avoid wasting arithmetic power, which provides useful reference for the management and use of high performance computing resources in colleges and universities.*

Keywords: *High performance computing, Colleges and universities, Repeated construction, Inadequate computing power, Security risks*

1. Introduction

High Performance Computing (HPC, also known as supercomputing) is a computer cluster system. The management node decomposes Computing tasks and assigns them to different Computing nodes to solve large Computing problems[1]. It is widely used in scientific research, simulation experiments, weather forecast, biopharmaceutical, gene sequencing, quantitative trading and other industries[2]. The development level of HPC is an important indicator of a country's scientific and technological strength and an important part of the national scientific and technological innovation system. The Outline of the National Medium- and Long-Term Science and Technology Development Plan (2006-2020) lists HPC as a key national development technology direction and a key information industry, and points out that it is necessary to strengthen the research and development of application software with independent intellectual property rights to ensure coordinated and balanced development with HPC[3].

The national supercomputing center is the basic service environment supporting all kinds of national scientific and technological computing and important engineering projects. It aggregates domestic excellent HPC resources and rich application software resources, and provides HPC and data processing services to users in various fields across the country through resource sharing. At present, China's supercomputing capacity ranks among the top in the world and has reached the P-level (1PFLops, trillion calculations). China's national Grid has been connected to seven national supercomputing centers.

2. Current situation of HPC in universities

With the increase of national investment in higher education, universities have made great progress in scientific research. It is precisely because of the improvement of scientific research level in colleges and universities, the demand for computing resources has grown rapidly in recent years, and more and more disciplines need to conduct in-depth research with the help of HPC resources. The HPC capability of universities will greatly promote the development of various disciplines. Therefore, more and more universities are building HPC centers[4, 5].

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2.1. The construction mode

Some colleges and universities have jointly established national-level HPC centers through cooperation with the government, and based on this, they have optimized the HPC ecological environment, implemented major application projects, cultivated HPC talents, and cultivated related strategic emerging industries. Among them, colleges and universities are mainly responsible for HPC center operation services, application development and personnel training, providing computer rooms, services and R&D sites, and employing operation service technicians and R&D talents. Some colleges and universities use self-built methods to build HPC centers, which provide a high-performance computing environment for talent training and technological innovation[6].

2.2. Existing problems

In-depth investigation of the needs and construction of HPC in some colleges and universities, it is found that most of the HPC resources in colleges and universities have the following problems.

2.2.1. Decentralized construction leads to waste of computing power

Although the total input of HPC resources in colleges and universities is very high in recent years, the maximum computing power that can be provided is not high. The root cause is that scattered input cannot achieve continuous superposition of computing power. Therefore, in the case of insufficient HPC resources, universities can only give priority to senior professors with strong research capabilities.

2.2.2. Decentralized construction leads to waste of computing resources

Due to the lack of unified HPC resource planning, the construction of HPC resources in some disciplines adopts the "project-driven" mode. After the project is completed, HPC resources are seldom used, which leads to the idle state of HPC computing resources, resulting in the embarrassing situation of "scarcity and waste" of HPC resources.

2.2.3. Repeated construction leads to waste of funds

Although many universities invest millions RMB in HPC every year, the lack of overall management leads to repeated construction of resources such as computer room environment, air conditioning, uninterrupted power supply, system and application software, resulting in a serious waste of funds.

2.2.4. Decentralized construction leads to waste of talents

Existing HPC resources are independently constructed by colleges, departments, and laboratories, which require a lot of time and cost in research, selection, and price comparison. These tasks that should be done by specialized technical personnel are usually done by high-end scientific researchers. As a result, a lot of scientific research energy of high-end scientific researchers is wasted.

3. Solutions to improve the utilization of HPC resources

The high performance computing system technology update cycle is short. If the machine is often idle and the usage rate is not high in the first five years, the investment cannot be recovered. Therefore, how to solve the problems of scattered computing resources, repeated construction, inadequate computing power, complicated operation and maintenance, and many security risks of HPC resource in colleges and universities, and give full play to the core potential of HPC platforms is an urgent task. The author provides the following two solutions for reference and research of universities.

3.1. Option 1: Building a university-level HPC center

3.1.1. The implementation plan

According to a series of factors such as the actual application requirements of HPC, the current computing scale, storage requirements, and calculation case size of various colleges on campus, a certain number of hardware and software devices are purchased to establish a high-performance computing platform environment which is highly scalable and easy to manage. Based on the principles of economy, energy saving and environmental protection, the HPC platform with multi-software/hardware support, multi-operation environment, unified user management, and multi-disciplinary scientific research application software operation is finally built through a

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step-by-step construction method.

3.1.2. Required software and hardware

The construction of university-level HPC platform mainly includes the construction of management/login node, computing node, storage system, network system and cluster management software. In the construction of high-performance computing environment, both software and hardware construction should be paid equal attention. In addition to buying hardware resources, major discipline software of each discipline should be purchased for the convenience of teachers and students' scientific research and achievements. Please refer to Table 1 for details.

Table 1: The hardware and software

serial number	Name	
1	management/login node	
2	computing node	regular compute node
		fat node
		GPU compute node
3	distributed storage system	
4	management network	Infiniband big switch
		Aggregation switch
		10 Gigabit Switch
		Gigabit switch
5	Cluster management software	
6	basic environment construction	Modular Data Center
		Power distribution system
		Cooling System
		Data Center Management System
		Computer room decoration
		Integrated wiring
7	Subject software	Gaussian
		VASP
		materials studio
		matlab
		COMSOL

3.1.3. Possible risks

Building a university-level HPC center is by no means the same as purchasing a set of high-performance computers. It also requires various systems and business construction to ensure service quality and efficiency. The construction of the HPC center is a coexistence of challenges and opportunities. The challenges are mainly reflected in three aspects: Can we give full play to the efficiency of the school-level HPC platform and solve the major disciplinary challenges faced by the school? Can the scientific research level of the school be significantly improved through multidisciplinary collaboration? Whether the sustainable development of the HPC platform can be achieved through high-quality services. It can be said that if the HPC platform is done well, it is a "multiplier" that promotes school development and career progress, and if it is not done well, it is a "money-burning machine".

3.2. Option 2: Integrate existing resources to establish university-level HPC center

3.2.1. Implementation Plan

Firstly, place the existing scattered HPC cluster resources centrally in the unified new server room of the university; secondly, the centralized HPC resources need to be connected together with computing nodes using unified network architecture and storage architecture; finally, the deployment and debugging of management software, scheduling software and application software are carried out in the physical cluster.

3.2.2. Possible risks

Completely seamless integration is difficult. The existing high performance equipment in the university have have varying performance due to different purchase times and limited funds at the time

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of purchase, and the hardware resources are updated quickly. Therefore, There's not much that can really be used after integration. Moreover, various damages may be caused during the handling process, so seamless integration may be an ideal situation.

In addition, the implementation of the program requires the cooperation of various departments. During the integration process, it is necessary to obtain the consent of the owner of the existing equipment, to contact with the manufacturer of each hardware device to obtain various parameters, and to negotiate with various departments of the university on many matters such as computer room land, power security, and network support.

3.3. Related safeguards

In order to provide users with a good scientific research environment, the university should continue to improve the basic environment, the management system, team building and funding guarantee in the operation and maintenance management system. The organic integration of the four ensures the safe, efficient and stable operation of the high-performance computing platform. Please refer to Figure 1.

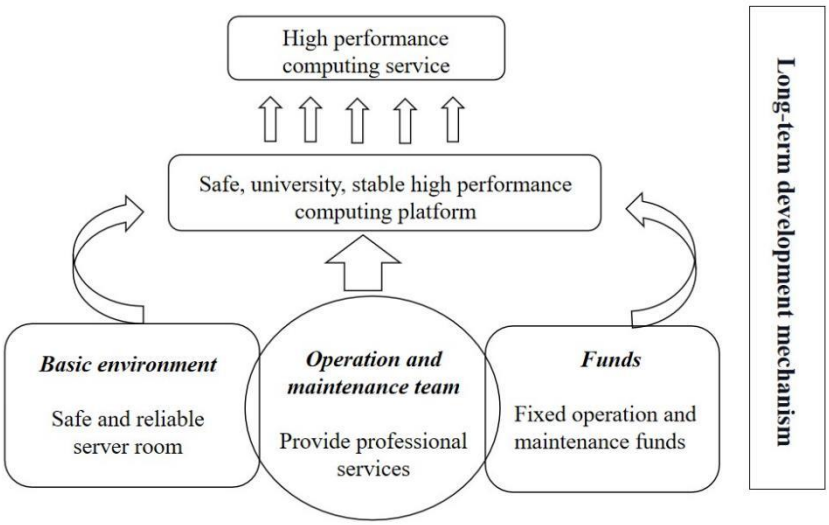

Figure 1: The management system of HPC platform

3.3.1. Basic environment guarantee

In the long run, a large independent computer room should be planned to build the supercomputer center. The school shall guarantee the basic conditions such as equipment room decoration, cabinet system, air environment system and refrigeration system, power supply and distribution system, dynamic environment monitoring and management system, fire control system, and network cabling.

3.3.2. Operation and maintenance team guarantee

Whether a HPC platform can run stably for a long time depends on the hardware and software resources it can provide on the one hand, and the services provided by managers for users on the other hand. The university should set up an independent department and establish a service and operation team to ensure the normal operation of HPC business.

3.3.3. Financial guarantee

After the establishment of the university-level HPC center, the university needs to continue to invest funds to ensure the efficient operation of the HPC center. First of all, fixed funds are provided every year to guarantee the maintenance and energy consumption of supercomputer center equipment. Secondly, if the campus resources are insufficient, new resources need to be purchased to improve the overall computing capacity of the platform.

3.3.4. Establish a long-term development mechanism

Implement a long-term development mechanism to promote university-level HPC. The sustainable development of HPC requires the active cooperation of various schools and departments. It is necessary to solve the problems in the system, policy and mechanism, and encourage the use of all parties

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through reasonable and effective mechanisms, so as to form a virtuous circle of self-development.

3.4. Advantages of the above schemes

First, centralized construction can effectively control decentralized investment. The university coordinates the planning and gives centralized investment to the university -level HPC center to solve the current problems such as scattered computing resources, repeated construction, inadequate computing power, complicated operation and maintenance, and many security risks.

Second, by establishing a high-performance computing platform, the university provides high-quality policies, resources and services to promote the introduction of talents and the construction of research teams, and helps the university to build a double-class.

Third, under the premise of reasonable integration of existing computing resources, the annual investment is precisely regulated according to the actual usage, and the limited funds are used for the expansion of the existing computing power, so as to realize the linear growth of the investment and the total computing power, and give full play to the efficiency of the use of funds.

Fourth, Centralized hosting solves the waste of computing resources, funds, talents, space and other problems caused by decentralized construction, provides a more professional guarantee for the construction, management and maintenance of computing resource environment, and effectively avoids the security risks caused by the poor computer room environment of each college.

Fifth, the sharing of resources can promote the harmonious development of disciplines. Breaking the barriers of exclusive resources of various colleges, departments, and laboratories, strengthening the radiation capability of HPC resources, ensuring that the existing scientific research teams can fully enjoy computing resources, and can also meet the high-performance computing needs of some teams and individuals who did not have the ability to purchase HPC resources before.

Sixth, Dedicated management can help to effectively improve the level of scientific research. According to the actual needs of each scientific research team for HPC resources, it provides professional technical support such as management and maintenance, and even assists the scientific research team to complete some research and development tasks, fully expands the coverage of scientific research, and promotes the training of HPC talents.

4. Conclusions

According to in-depth research and analysis, combined with the current situation of various universities, the above two solutions can be used alone or in combination to solve the problem of scattered HPC resources and unified supervision in colleges and universities. If the on-campus resources are not enough to meet the scientific research needs of some teachers and students, the resources of the national HPC center can also be introduced as a supplement to the on-campus platform resources. According to HPC research, many companies in the industry can customize the exclusive HPC cloud desktop for each university and connect with the university's unified account management and authentication system. Teachers and students can quickly use the computing resources of multiple national HPC centers by logging in to the HPC cloud platform with the account of the school's unified portal. The construction and management of high performance computing in in colleges and universities is not only a problem of information technology, but also a problem of management. Due to the limited level of the author, I would like to draw on this, hoping that more colleagues engaged in high performance computing can summarize the construction, operation and management experience of high performance computing, to learn from each other's strengths and shortcomings.

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