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STUDY AND DESIGN OF THE APPROPRIATE HIGH-PERFORMANCE COMPUTING SYSTEM FOR BEAMLINE DATA ANALYSIS APPLICATION AT IRANIAN LIGHT SOURCE FACILITY (ILSF)*

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Abstract

Data analysis is a very important step in doing experiments at light sources, where multiple application and software packages are used for this purpose. In this paper we have reviewed some software packages that are used for data analysis and design at Iranian Light Source Facility then according to their processing needs, after taking in mind different HPC scenarios a suitable architecture for deployment of the ILSF HPC is presented. The proposed architecture is a cluster of 64 computing nodes connected through Ethernet and InfiniBand network running a Linux operating system with support of MPI parallel environment.

INTRODUCTION

To do research on the structure of different materials, we can study the structure of materials at the level of its atoms. Active synchrotron light sources around the world study the structure of materials using X-rays in beam lines. Techniques used in beam line experiments can be divided into absorption, diffraction, emission or reflection, imaging, ion spectroscopy, lithography, photoelectron emission and scattering. The data generated and recorded through these experiments need to be analysed in order to obtain useful information from this raw data. Several applications have been developed to perform these analyses and are used by synchrotron light sources. Analysing this data by researchers is time consuming, depending on factors such as the hardware used and the amount of data processed.

Computing plays a key role in synchrotrons. In particular, advanced software plays an important and influential role in the performance and efficiency of operations and experiments performed on beam lines in synchrotron assemblies. According to previous studies in this field, with the increase in data production rate, the importance of using advanced software to provide timely results has become more apparent. The use of advanced and new data analysis software as well as the implementation of appropriate computing infrastructure is one of the important needs of users and researchers in synchrotron collections [1].

Data analysis requires high-performance computing to achieve results in short time, as well as the use of technologies such as multi-threaded processing and convenient graphics processors [2]. According to the mentioned cases, identifying suitable software for analysing the data generated by performing various experiments in beam lines, as well as the hardware requirements of each, including the required memory, number of processors, graphics card etc. is necessary. This paper examines the hardware requirements for analysing beam line data as well as some of the software used to analyse the data generated in ILSF beam lines.

HARDWARE AND COMPUTATIONAL NEEDS FOR ANALYSING THE DATA PRODUCED IN EXPERIMENTS AT ILSF BEAMLINES

In general, the analysis of data obtained through experiments at beam lines of the light source can be done in two ways. In the first method, the data obtained is first stored in external storage and then analysed at another time. In this method, due to the large volume of data generated, external storage with notable capacities is required. In the second method, which is done in real time, it is necessary to use supercomputers or processing systems with high computing power [3].

In general, there are four hardware components that should be considered for data analysis and simulation using various software used at the beam lines, including Avizo, TomoPy, HLK2000, FIT2D, HipGISAXS, XMAS and MIDAS. These four components are: graphics card, processor, main memory and external storage. The necessity of each of them is stated below [4].

Graphics Card

The volume of data produced in ILSF collections is increasing day by day. Due to the extensive developments in the field of laboratory tools, including detectors, cameras, etc., the generated data have a high quality and volume. The performance of various software in image processing, in addition to the CPU, depends on the graphics card used. Different GPUs may be used depending on the test performed and the software used. GPUs also differ in the amount of memory they have. The minimum recommended memory for a GPU is 1 GB, but the most powerful GPUs have between 12 and 16 GB of memory. Choosing a GPU with the right memory depends on the amount of data being processed.

Some analytics software used in beam lines, such as Avizo, do not care much about the type of GPU, but only

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that the GPU used can fully implement the OPENGL 2.1 or higher. This is while some other software requires a special version of GPUs.

Processor

As mentioned, computing plays a key role in the analysis of light source beam line data. The main processor is one of the hardware components that is important to pay attention to. Depending on the different computational needs of data analysis software, processors with different specifications are used. Today, due to the high volume of data generated through various experiments, the need for real-time analysis and data reduction techniques is felt. With advances in laboratory equipment, including detectors, leading to high-quality, high-volume image data in beam lines, the use of a single processor, even multi-core, is not very efficient, and this is exactly where the importance lies. The use of multi-core multiprocessor systems, computing clusters and even grid computing systems is emerging.

Memory

Another important hardware component in analysing the data generated by performing various experiments at beam lines is main memory and external storage. Various data analysis software packages need high-capacity main memory to minimize latency in order to be able to analyse large volumes of data very quickly. Also, after the data is analysed, memory with the appropriate capacity is needed to store the results of the analysis. When data processing and analysis is not real-time, high-speed and high-capacity storage is also needed to minimize latency due to data transfer between storage and main memory.

PROPOSED HPC DESIGN

In this section, according to the computational needs of different data analysis software and the possible rate of data production in each beamline of the first stage of launching Iranian Light Source Facility, a high-performance computing system to perform the calculations required by data analysis software is suggested. In addition to periodic upgrades, the hardware and software of this system must be upgraded and improved by increasing the number of beamlines.

For the following reasons use of cluster computing is recommended:

- Has a lower implementation cost than performance.
- The price of hardware and software is reasonable and relatively low.
- The cost of supply and maintenance is low.
- It is possible to develop and update the system at a relatively reasonable cost.
- The system development can be done easily by increasing the need.
- If necessary, it is possible to use this system in the form of a grid system or cloud.
- Most high-performance computing systems use this type of architecture.
- A number of synchrotrons including Diamond light source and Sesame also use cluster computing for their calculations.

Proposed Computing Cluster Hardware and Software

One of the types of clusters that have different applications in meteorological systems, seismography and various sciences is the Beowulf cluster which has a relatively good performance. This type of class has a simple architecture that consists of a server node and several computational nodes and a network for communication between nodes.

The type of hardware of the server node and computing nodes, the type of network technology, the operating system and the type of programming model of the proposed cluster are given in Table 1.

Table 1: The Type of Hardware and Software Used in the Proposed Cluster

Item	Specification
Server type	Dell PowerEdge R710 (Better or Similar one available at the implementation time)
Server CPU type	Intel Xeon (Better or Similar one available at the implementation time)
Server Memory	32 GB
GPU	NVIDIA TESLA K20 (Better or Similar one available at the implementation time)
Computing node	64
Computing node CPU type	CPU intel core^{TM} i7 (Better or Similar one available at the implementation time)
Per node memory	128 GB
Hard disk capacity for server	2 TB
Hard disk capacity for each node	1 TB
Network	10 Gigabit Ethernet + InfiniBand
Operating System	Linux
Parallel Environment	MPI

In the following, a brief explanation is given about each of the selected hardware and software components for the proposed system and the reasons for choosing each one.

Server and Computing Node The processors used in the design of the proposed cluster are processors made

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by Intel. The operator of this cluster has an 8-core Zeon processor that has good computing power. Also, 32 GB of main memory or RAM is provided for this server. In addition to the 8-core Zeon processor, the server is also equipped with NVIDIA Tesla graphics cards. According to the type of possible experiments and the approximate estimate of the volume of production data in the seven beamlines of the first stage of launching ILSF, currently 64 computational nodes have been considered for this computational system. Naturally, the number of nodes can be changed as this information is updated. The current number of cores per node is 32 cores, but due to technology upgrades and lower cost of processors with more cores, this number can be increased during the actual implementation.

In this case, assuming a constant budget, a compromise can be made between the number of nodes and the number of cores per node. More nodes contribute to the redundancy of this computing system. More cores in a node allows the processing of data through the high-speed internal bus of that node and by imposing less load on the Gigabit network or INFINIBAND computing cluster. In cluster implementation for proper use of processing resources and optimal performance, a minimum of 4 GB of RAM per core is recommended.

Network Technology Another key component in computing cluster design is its network technology. Given that the computing system must be able to have acceptable computing power, the connection between the nodes of the computing system, which can be the bottleneck of the performance of this system, is of particular importance. Considering current needs and to maintain flexibility and scalability in responding to new needs, there must be a rapid internal connection between cluster nodes. One of the most widely used networking technologies is Gigabit Ethernet technology, which is also used in most computing clusters, including those used in the Diamond Light Source. This technology has a high data transfer rate and low latency. Having the ability to communicate through INFINIBAND, provides more redundancy and the possibility of communication with less latency than Gigabit Ethernet. It is recommended to have this feature in applications where there is a lot of storage and processing load at the same time

Operating System The proposed operating system for this cluster is the Linux operating system. The reason for choosing the Linux operating system is that it is an open-source operating system and is easily and freely available to consumers. Most beam analytics software also supports this operating system. Also, this operating system is well compatible with Gigabit Ethernet network technology.

Programming Model MPI is a standardized message-passing interface designed by a team of academic and industrial researchers to work on a wide range of parallel computers. Due to the widespread use of this parallel programming communication contract in analytical software with parallel processing capability, providing the possibility of developing and executing such programs requires the implementation of MPI in the computational cluster system.

CONCLUSION

For analysing the data produced in experiments at ILSF beamlines, the general need includes hardware components like graphics card, processor, main memory and external storage. The pertinent hardware components were considered for data analysis and simulation using various software used at the beamlines. The SMP (Symmetric Multi-Processor), Cluster Computing, and also Grid Computing, are the different HPC (High Performance Computing) scenarios that were studied. Finally, a suitable HPC design is proposed for responding the beamlines data computational requirements of the ILSF's future beamline scientists.

REFERENCES

[1] PaNdata Software Catalogue, `https://software.pan-data.eu/software`

[2] THE home for Small Angle Scattering, `http://smallangle.org/content/software`

[3] S. T. Chourou, A. Sarje, X. S. Li, E. R. Chan, and A. Hexemer, "HipGISAXS: a high-performance computing code for simulating grazing-incidence X-ray scattering data", *Journal of Applied Crystallography*, vol. 46, pp. 1781–1795, 2013. doi:10.1107/S0021889813025843

[4] *The HKL-2000 Manual, Edition 2.6*, HKL Research, Inc., Charlottesville, VA, USA, 2007. `https://hkl-xray.com/hkl-2000-manual`