Activities for HPC ISV Applications

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Computer simulations for research and development are performed widely in universities, institutes and industries. For these simulations, High Performance Computing (HPC) platforms are often used and various overseas and domestic Independent Software Vendor (ISV) applications are also used. Therefore, Fujitsu promotes enabling and optimization of ISV applications for Fujitsu's HPC platforms and provides troubleshooting support for customers who use ISV applications on Fujitsu's HPC Platforms, and by arranging five ISV application support bases, Fujitsu has given such support with a global support formation.
This paper introduces Fujitsu's HPC platforms as well as the performance characteristics of HPC ISV applications, the details of customer support and the support formation for HPC ISV applications.

1. Introduction

Since the launch of Vector Processor FACOM VP-100/FACOM VP-200 in 1982, Fujitsu has been supplying High Performance Computing (HPC) platforms. These platforms have been used for various simulations in scientific and engineering areas such as structure analysis, fluid analysis and crash analysis. Motivated by recent improvements in platform performance and development of simulation technologies, simulations are widely used now as a powerful tool for research and development. For these simulations, various overseas and domestic Independent Software Vendor (ISV) applications are used frequently. To address these trends, Fujitsu has been providing HPC platforms with a global support formation for ISV application users.

The following sections describe the Fujitsu's activities for HPC ISV applications.

2. Fujitsu's HPC platforms

Currently, Fujitsu supplies a PC cluster system and a large-scale Symmetric Multi Processing (SMP) system as HPC platforms. Fujitsu also supplies a SPARC64-processor-based server called FX1 that is specialized for use in high-end technical computing. The PC cluster system has excellent cost efficiency and high expandability. On the other hand, large-scale SMP systems can integrate high-capacity memory with high I/O throughput, making them suitable for applications that require such capabilities.

Fujitsu's PC cluster system and large-scale SMP system are briefly outlined below:

1) PC cluster system

High-performance cluster system in which the high-performance, high reliability PC server PRIMERGY/high performance technical computing server HX600 is used as a computational node and combined with a high-speed interconnect.

- CPU: Intel Xeon processor (PRIMERGY)
  AMD Opteron processor (HX600)

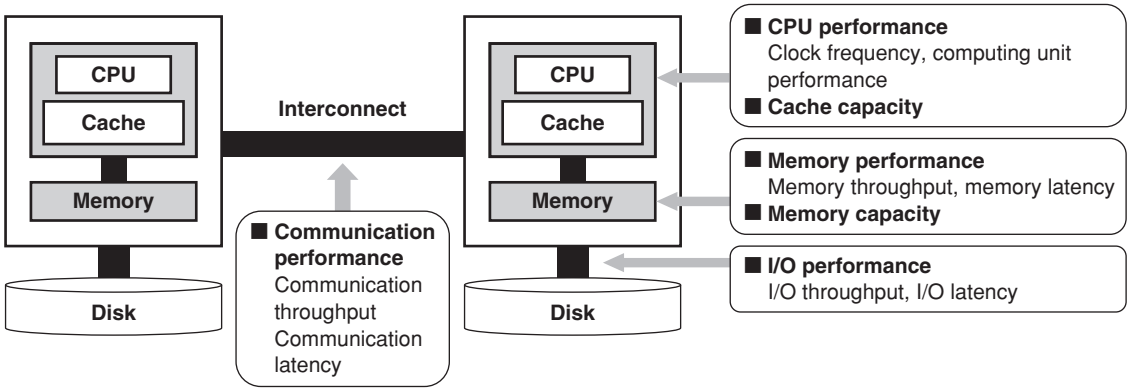

Figure 1
Main hardware factors which influence application performance.

- OS: Red Hat Enterprise Linux
- Interconnect: InfiniBand etc.

2) Large-scale SMP system

As large-scale SMP systems, the mission critical IA server PRIMEQUEST, which is the most powerful open server in the world, and the global standard UNIX server SPARC Enterprise are available.

- PRIMEQUEST
  CPU: Intel Itanium processor
  OS: Red Hat Enterprise Linux
- SPARC Enterprise
  CPU: SPARC64 processor
  OS: Solaris

PRIMEQUEST and SPARC Enterprise can take cluster configuration by using InfiniBand etc.

As HPC middleware for the PC cluster system and large-scale SMP system, Parallelnavi is available. Parallelnavi ensures HPC language system and job/system management, and our abundant experience with Fujitsu's supercomputer VPP Series and PRIMEPOWER HPC2500 have been extended and are reflected in it. Its functions are described below:

- Operation management (job scheduler, HPC enhancement, HPC cluster management)
- Language system (compiler, library, development tool)
- High speed network file system (SRFS: Shared Rapid File System)

3. HPC ISV applications

While HPC ISV applications are currently often used for structure analysis, fluid analysis and crash analysis, use of computational chemistry applications is expected to increase in future in the field of nanotechnology and life science.

High-speed execution is required for HPC ISV applications. Therefore, it is essential to choose suitable hardware depending on the performance characteristics of the application. In the following section, the hardware factors that influence the sustained performance of ISV applications are described.

1) Application performance and hardware

Factors that influence the computation speed of an application are not only CPU performance but also memory performance, I/O performance and interconnect communication performance. **Figure 1** indicates the factors that influence the sustained performance of an application.

- CPU

CPU clock frequency and configuration of the arithmetic unit such as computational pipeline, Single Instruction, Multiple Data (SIMD) are important. Also, CPU cache capacity influences the performance.

- Memory

The memory throughput performance between memory and CPU and memory latency at memory access are important. Further,

Table 1
Application characteristic for each analysis area.

Analysis area	Application characteristics[note 1)]				Hardware factors that influence application performance	Fujitsu platform suitable for application
	Within single node			Parallel effect		
	CPU load	Memory access load	I/O load			
Structure analysis	High	Mid to High	Mid to High	Low	CPU performance Memory performance Memory capacity I/O performance	PRIMEQUEST/ SPARC Enterprise
Fluid analysis	Mid	High	Low	High	CPU performance Memory performance Communication performance[note 2)]	PRIMERGY/HX600 cluster + High-speed Interconnect (InfiniBand)
Crash analysis	High	Mid	Low	High	CPU performance Memory performance Communication performance[note 2)]	PRIMERGY/HX600 cluster + High-speed Interconnect (InfiniBand)
Electromagnetic wave analysis	Mid	High	Low to Mid	High	CPU performance Memory performance Communication performance[note 2)]	PRIMERGY/HX600 cluster + High-speed Interconnect (InfiniBand)
Computational chemistry (Molecular orbital method)	Mid	Low to Mid	Low to High	Low to Mid	CPU performance I/O performance	PRIMEQUEST/ SPARC Enterprise

note 1) While the application characteristics depend on the analysis details, the table above indicates their general tendency.
note 2) Communication performance is influential during the highly parallel execution of PC cluster system.

some applications generate a large amount of I/O and in such case, integrated memory capacity may have significant influence on the sustained performance of application, because the memory is used as I/O cache.

- I/O

The I/O throughput performance to disk unit and I/O latency at disk access are important.

- Interconnect

The communication throughput performance between nodes and communication latency at inter-node communication are important. In the case of cluster configuration, an increase of computation nodes leads to an increase of ratio of communication time compared with computation time. For this reason, the importance of communication performance will increase and a high-speed interconnect is indispensable. Currently, InfiniBand is widely used as a high-speed interconnect. InfiniBand can be used on Fujitsu's HPC platform.

2) Performance characteristics of applications

Table 1 indicates the performance characteristics of applications used in typical analysis fields and shows the Fujitsu HPC platform suitable for each analysis field.

The characteristics of applications used for structural analysis are higher I/O load and smaller parallel efficiency in comparison with ones of fluid analysis and crash analysis. Therefore, a large-scale SMP system is suitable for executing applications of structural analysis. Meanwhile, because applications of fluid analysis and crash analysis indicate a high parallel efficiency and low I/O load, PC cluster is a suitable system considering cost-efficiency.

Further, in the field of fluid analysis, memory access performance tends to be a bottleneck, because its memory access load is high.

Thus, it is important to pay attention to the characteristics of each application when selecting a suitable platform.

4. Fujitsu's activities for ISV applications

Fujitsu promotes enabling and optimiza-

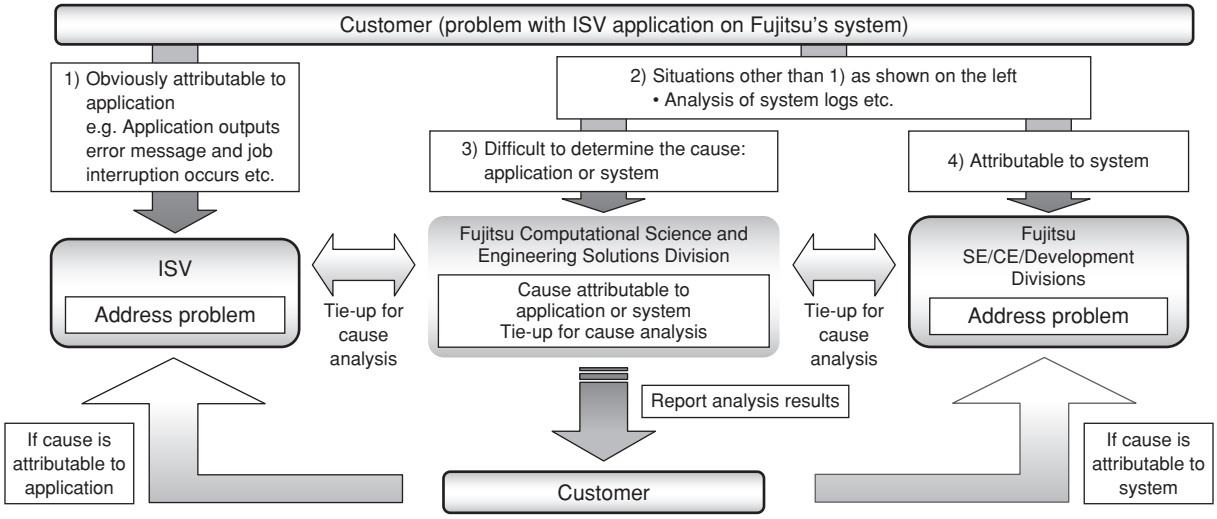

Figure 2
Support formation for ISV application problems.

tion of HPC ISV applications for Fujitsu's HPC platforms and provides troubleshooting support with a global support formation for ISV application users on Fujitsu's HPC platforms.

1) Promotion of enabling and optimization for Fujitsu's HPC Platforms

Customers request to use various ISV applications. To address these requests, it is essential to enhance the variety of ISV applications available on Fujitsu's HPC platforms. To achieve this, Fujitsu promotes enabling of ISV application for Fujitsu's HPC platforms with the cooperation of domestic and overseas ISVs.

Further, performance characteristics such as CPU load and memory access load are analyzed for typical ISV applications on Fujitsu's HPC platforms. These analyses are fed back to hardware and software development divisions for further improvement of the performance of Fujitsu's HPC platforms.

2) Troubleshooting support for ISV application users

With the cooperation of ISVs, Fujitsu is providing troubleshooting support for Fujitsu system users who are faced with problems related to ISV applications.

Figure 2 shows Fujitsu's actions regarding trouble related to ISV applications. When the problem obviously comes from the application, the ISV will directly address the issue. When the problem obviously comes from the system, Fujitsu will address the issue. However, in many cases, it is difficult to identify whether the problem comes from the application or the system. Adequate knowledge of both ISV applications and the system is needed for an appropriate breakdown of the cause of the problem in such cases. Therefore, Fujitsu's ISV application support team is offering a service of appropriately identifying the cause of problems to ensure prompt solutions, in a close tie-up with domestic and overseas ISVs and Fujitsu's hardware and software development divisions.

3) Support formation

Many HPC ISV applications are developed by overseas ISVs. For this reason Fujitsu has arranged support bases in the United States, Europe and Australia in addition to the domestic base, establishing a global support formation. This formation allows Fujitsu to offer support under close tie-ups with domestic and overseas ISVs. The following five locations are the support bases for the activities mentioned above (**Figure 3**).

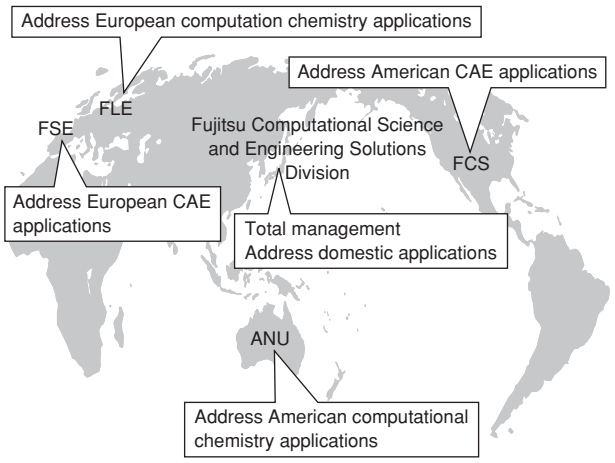

Figure 3
Site for ISV application support.

- Japan (Chiba): Fujitsu Computational Science and Engineering Solutions Division

This site manages whole Fujitsu's activity for HPC ISV applications and addresses the issues related to ISV applications developed in Japan such as SCRYU/Tetra.

- USA (San Jose): Fujitsu Computer Systems Corp. (FCS)

This site addresses the issues mainly related to CAE applications developed in the United States such as LS-DYNA, FLUENT and Nastran.

- France (Toulouse): Fujitsu Systems Europe Ltd. (FSE)

This site addresses the issues mainly related to CAE applications developed in Europe such as PAM-CRASH, RADIOSS and STAR-CD.

- UK (London): Fujitsu Laboratories of Europe Ltd. (FLE)

This site has sophisticated knowledge about the computational chemistry applications developed in Europe, addressing the issues related to computational chemistry applications such as Molpro and Molcas. Also, it addresses the UK-made math library NAG.

- Australia (Canberra): The Australian National University (ANU)

With its high level of technology in the area of computational chemistry, this site addresses the issues related to computational chemistry applications developed in the United States such as Amber, GAMESS-US and Gaussian.

In recent years, requests to hold seminars on how to use computational chemistry applications have arisen from customers mainly in the academic community. To address such requests, Fujitsu holds seminars in cooperation with ANU researchers.

5. Conclusion

This paper described Fujitsu's HPC platforms as well as the performance characteristics of HPC ISV applications, details of customer support and the support formation for HPC ISV applications.

To support HPC ISV application users, Fujitsu promotes enabling and optimization of HPC ISV applications for Fujitsu's HPC platforms and provides troubleshooting support, establishing a global support formation.

To address customers' various needs for ISV applications, Fujitsu will also develop and provide new solutions and services in future to contribute to the promotion of the research and development activities of the customers.

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Mr. Fukunaga received the B.S. and M.S. degrees in Physics from Tsukuba University, Ibaraki, Japan in 1990 and 1992, respectively. He joined Fujitsu Ltd., Tokyo, Japan in 1990 and has been engaged in support and promotion of Fujitsu's High Performance Computing (HPC) System.