

Approach to Utilizing High-performance Computing at HPC Wales

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HPC Wales has been providing high-performance computing (HPC) infrastructure to enterprises and universities in target domains for future business development, research innovation and nurturing of human resources. This project is carried out by HPC Wales in collaboration with the UK government, Welsh government, EU and Fujitsu. In particular, Fujitsu has provided HPC system infrastructure, transferred knowledge and collaborated in research with HPC Wales. In this paper, we describe the HPC infrastructure in HPC Wales and its approach to utilizing HPC technology for business development.

1. Introduction

In the field of large-scale simulations, High-performance computing (HPC) is a technology that to date has been mainly used for scientific computing in universities and research institutions. Recently, HPC technology has come to be applied in an increasing variety of fields. In addition, computers have become further commoditized as represented by the x86 architecture, and this has made it possible to provide an HPC system at a lower cost than ever before. For that reason, organizations can now use such a system through a cloud environment without having their own computing resources. Furthermore, large enterprises and research institutions, and organizations that were unfamiliar with HPC in the past have come to benefit from the technology.¹⁾ Application fields have widened, with finance and social infrastructure, including smart communities, recently adopting HPC technologies, not to mention R&D fields such as product design, meteorology, aerospace and bioscience.

Based in Wales in the UK, HPC Wales,²⁾ is a public-service corporation that is focused on the industrial application of HPC technology. It is operated by a not-for-profit organization consisting of universities belonging to the St. David's Day Group and the University of Wales. HPC Wales has supercomputers at three different scales—"large", "medium" and "small"—distributed amongst Welsh universities, with the major

production systems in Cardiff and Swansea Universities.

It provides computing resources that allow users to make use of the HPC technology as required. It also aims to revitalize local industries through utilizing supercomputers, in addition to promoting R&D and fostering IT human resources, by disseminating HPC technology among universities and regional enterprises. With a total budget of 40 million pounds, this national project will both establish and fully exploit the associated HPC infrastructure by 2015.

In January 2011, HPC Wales appointed Fujitsu as a partner for the project (announced in April 2011)³⁾ and we are jointly moving ahead with the project in order to accomplish its purpose. This paper outlines the distributed HPC system introduced in the project and describes the approach taken by HPC Wales and Fujitsu to promoting its usage.

2. Fujitsu's major activities in HPC Wales

Major activities carried out by Fujitsu in the collaborative project with HPC Wales include:

- 1) Provision of HPC system infrastructure

HPC clusters capable of a total of 320 TFLOPS are deployed in eight universities distributed across Wales to provide an open and easy-to-use environment that allows users to readily access the HPC resources.

2) Promotion of use and dissemination activities

This activity aims to foster HPC specialists and disseminate its technology to users. HPC Wales and Fujitsu have been cooperating with business consultants and HPC vendors to provide support for its activities through education, training and consulting.

3) Research collaboration

Researchers at universities in Wales and regional enterprises are engaged in research collaborations in mutual partnerships established to create new capabilities. They have been working to continuously produce practical outcomes through partnerships with private enterprises. At present, HPC Wales oversees some 80 research projects of varying themes, with many more in the pipeline. Fujitsu is assisting with some 25% of these, the details of which will be outlined in the section 5.

3. System infrastructure supporting HPC Wales

3.1 HPC cluster system

As shown in **Figure 1**, eight of the universities in Wales are classified into the three categories of "Hub", "Tier 1" and "Tier 2". These are host to the so-called "large", "medium" and "small" operational PC cluster systems respectively. In the Hub category, which hosts large-scale clusters, Swansea University is classified as Hub A and Cardiff University as Hub B. The Tier 1 sites, with medium-scale clusters, include the Universities of Aberystwyth, Bangor and South Wales, while Swansea Metropolitan University, Glyndwr University and the Bridge Innovation Centre (BIC) are Tier 2 sites, each with small-scale clusters. The cluster systems are based on FUJITSU Server PRIMERGY BX900 series and CX400 series—Fujitsu's PC servers—and feature more than 1000 nodes in total, with large-scale storage systems.

The systems implementation in Phase 1 of the project was completed between July 2011 and December 2012. In this phase, eight clusters in total were installed, including two clusters in Hub B, and a single cluster at each of the three Tier 1 and three Tier 2 universities—all based on Westmere processors. The clusters at each site are connected to a high-speed network and have shared storage to house user data. In the Hub clusters, parallel file systems which adopt Lustre technologies are available, used for processing intermediate files during job execution.

The implementation of HPC Wales Phase 2 was completed in August 2013, delivering an additional six clusters in Hub A and Hub B, all based on Sandy Bridge processors.

3.2 Infrastructure software

1) Use of Cluster Manager

A PC cluster is an HPC system in which a large number of PC servers having similar configurations are used as computing nodes, mutually connected via a high-speed network, to deliver high-speed computing through parallel processing. Expecting engineers to manually set up individual servers is both inefficient and demanding in both time and resources, involving an excessive amount of work, including the installation of software, plus the configuration and maintenance during system operation. Accordingly, Fujitsu has provided HPC system management software whereby an administrator can manage individual components of the cluster from a single management node.

2) Dual-boot cluster

The High-Throughput Cluster (HTC) system provided in Cardiff University has delivered a Linux/Windows dual boot function. With this in place, a user may specify the desired OS environment using the job scheduler option in the job execution script such that the operating system automatically switches between Linux/Windows given available resources, and the job can be executed on the specified OS.

3) Application execution platform

In executing an application, it is necessary to set up the required software environment before job execution. However, different products use different compilers, libraries and middleware and changing the required environment each time according to the application poses a burden on end users. To deal with this problem, we have established an environment in which a user can select the job execution environment from an application list, enabling users to easily import the necessary build and job execution environment according to the application.

4) HPC Gateway

The project aims to provide an environment that allows regional enterprises and students without expertise in HPC to exploit fully the available HPC resources. For that reason, a job execution environment—the HPC Gateway—is provided through which an intuitive user

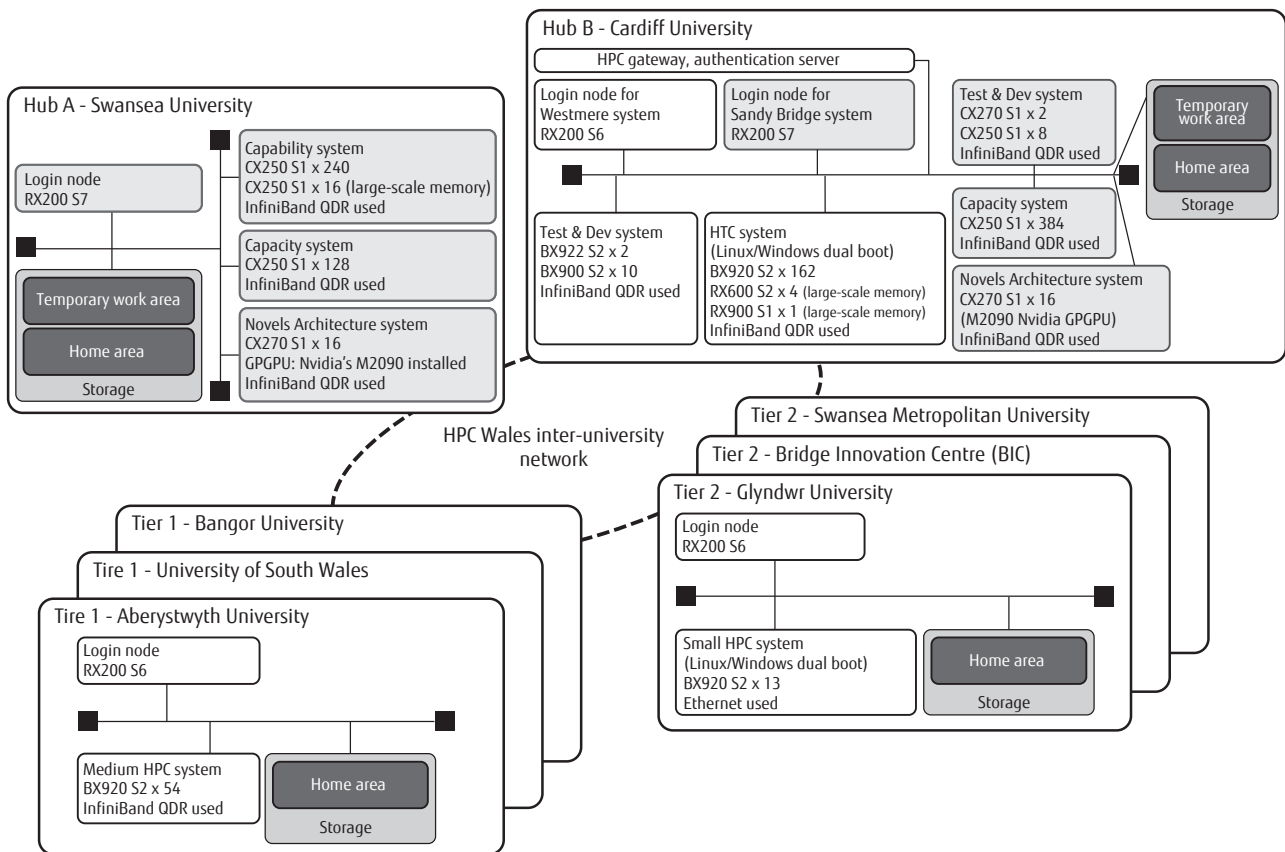


Figure 1 Overview of HPC cluster structure in HPC Wales.

interface can be used to allow transparent use of distributed HPC resources.

The dedicated client or a Web browser installed on the end user's PC is used to access the HPC system from a screen. In the future, we intend to provide the capability of building continuous operations, such as a parametric survey, into a flow for batch processing.

Figure 2 shows an image of using the dedicated client. The end user launches the dedicated client introduced in the PC. For simulation, an application execution file registered on the left side of the screen is selected. Then, after specifying the necessary input, output and execution parameters, a job is submitted, which automatically transfers the necessary files and selects the available resources from multiple PC clusters for executing the job. When the execution has been completed, the analysis result is automatically transferred to the predefined directory on a storage device.

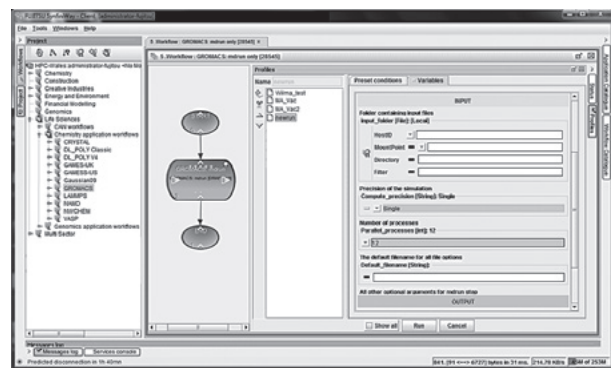


Figure 2 Analysis execution screen of HPC Gateway.

4. Promotion of use and dissemination activities

4.1 Holding of workshops (Outreach)

As part of outreach activities, HPC Wales and Fujitsu regularly hold workshops for disseminating HPC and promoting use of HPC by regional enterprises.

Through this activity, HPC Wales introduces HPC technology and the benefits of use of HPC, presents practical examples of related vendors and venture enterprises and offers opportunities for consulting and a case study on how HPC can be utilized in real-world operations. It also introduces the services and computing resources that are offered by HPC Wales and demonstrates the use of HPC usage environments.

These represent excellent opportunities for HPC Wales to clarify the services and necessary support to be offered in the future, communicating with existing and prospective users through the recently formed HPC User Group.

4.2 Education activities (Skills Academy)

When using HPC resources, even those familiar with computer operations in their day to day activities need to learn basic operations such as the use of the software development environment, execution of simulation using HPC resources, pre- and post-processing including mesh creation and data extraction. HPC Wales and Fujitsu partner with the Numerical Algorithms Group (NAG) of the UK—a well-known independent software vendor—to provide this insight. While currently based on regular lectures, adopting hands-on training and remote education by e-learning is about to be launched through the HPC Wales Learning and Management system (LMS).

5. Research collaboration

5.1 Optimization of application execution environment

NAG and Fujitsu Laboratories of Europe (FLE) are working in collaboration to carry out support activities including the optimization of key applications required for the research mentioned earlier and promotion of HPC use.

1) Application benchmark

In partnership with FLE, HPC Wales has selected prominent applications from current research projects to study scalability premised on parallel processing, CPU, memory, I/O and other application profiles.

2) Establishment of general-purpose technologies for benchmarking

Performance analysis tools and the associated profiler utilization technology for studying application characteristics have been put in place to build an

environment that allows non-expert users to readily gain an understanding of application characteristics by using established and proven methodology.

3) Application to real systems

An understanding of application characteristics makes it possible to decide which application is suitably used in which machine environment. Across the HPC Wales infrastructure, various machine environments are available including large symmetric multiprocessing (SMP) computers and high-speed storage devices, in addition to clusters at different scales of large, medium and small. In such a mixed-device environment, executing applications with low scalability at a high processor count or executing non-memory-intensive jobs by using a large SMP computer is inappropriate and are factors that hinder the efficient use of resources.

In order to solve these problems, we aim to build a support environment that allows execution of jobs in an appropriate environment based on the results of 1) and 2) above.

5.2 Creation of new technologies

In addition to the above, 20 research projects have been started as collaborative ventures. The major fields of activities include life science, energy and meteorology and advanced materials and manufacturing. These are intended to create new capabilities based on a scholarship system for young researchers and for HPC dissemination activities (education in the use of HPC and consultation for business use of HPC for Welsh enterprises). For this reason, joint activities with regional enterprises in Wales are an essential requirement for accepted research projects.

1) Energy

In the coastal area of North Wales, use of tidal power generation to meet part of future energy demand is raising expectations. Related research includes that on the design of a tidal turbine system and verification of the effectiveness of tidal power generation off the coast of Wales.

2) Environment

In order to identify CO₂ emissions caused by droughts in Welsh peat bogs, research is underway to clarify the ecological mechanisms and work out the port development design by using 3D ocean models for studying the relationship between sedimentary sand

and tidal currents.

3) Life sciences

In the field of life sciences, research is conducted on second-generation DNA sequencing devices capable of reading the whole genome sequence at a very high speed and low cost.

4) Meteorology

Wales, which is naturally subject to changeable weather, suffers frequent floods and river overflows, and these have a great impact on neighboring residents. Research is in process to build a system that carries out simulation of such abnormal weather for working out appropriate countermeasures.

As of September 2013, twenty projects have been selected out of the fifty submitted for application, with the ensuing research activities already leading to significant impact.

6. Conclusion

This paper has presented the example of HPC Wales as an overseas HPC customer of Fujitsu, focusing on the fields in which HPC technology is used and its intended effects. This example clearly shows that the application of HPC extends beyond the academic fields of science and technology, into the field of society in which we live, a field in which the successful adoption of technology is expected to lead to successful results and resultant impact. In the future, it is thought HPC

will permeate into private enterprises including the manufacturing industry, increasing the likelihood of its uptake by developing countries.

Meanwhile, there is still only a small pool of human resources capable of using the HPC technology freely and sufficient education for use of HPC, analysis on which part of which operation can make the most of the technology and adequate study of its effect are necessary.

The number of HPC projects is expected to continue to increase overseas as well as in Japan. The point seems to be how to most effectively use the system infrastructure that is introduced.

To further enhance the contribution of HPC to society, Fujitsu is committed to continuously providing products and solutions capable of solving various problems of society.

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